Locality of Interatomic Interactions

PDE Seminar, UMN

Jack Thomas

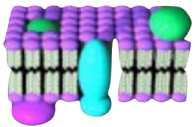
Joint work with Huajie Chen (Beijing Normal University)
and Christoph Ortner (University of British Columbia)

slides: https://z.umn.edu/JT-notes

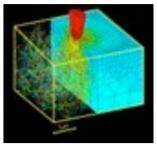
UNIVERSITY OF MINNESOTA

Motivation

Abstract: *"We survey some recent results on the sparsity of the potential energy landscape (PEL) aimed to justify and extend the theory of machine-learning for interatomic potentials"*



Coarse grained molecular

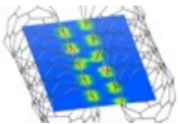


Interatomic potentials

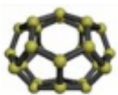
E^{IP}

E^{QM}

Empirical QM



Density Functional Theory (DFT)



Quantum Monte Carlo

Quantum Chemistry

Accuracy

System size / timescale

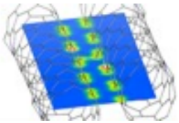
[Image courtesy of Gábor Csányi]

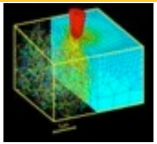
Goal: (Qualitative) justification for the assumptions made in interatomic potentials

Proof: Polynomial approximation

Accuracy

E^{QM}





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Density Functional Theory (DFT)

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System size / timescale

Outline

Density Functional Theory

- Many-body Schrödinger equation: $\mathcal{H}_{\mathrm{tot}}\Psi = E\Psi$

KS DFT

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- Many-body Schrödinger equation: $\mathcal{H}_{\mathrm{tot}}\Psi = E\Psi$
- Born–Oppenheimer: solve for the electrons $\mathcal{H}_{\mathrm{BO}} = \mathcal{H}_{\mathrm{BO}}(\boldsymbol{r})$
  [where $\boldsymbol{r} = (\boldsymbol{r}_1, \ldots, \boldsymbol{r}_{N_{\mathrm{at}}}) \in (\mathbb{R}^d)^{N_{\mathrm{at}}}$]

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KS DFT

$$\mathcal{H}^{\mathrm{KS}}\psi_i(x) \coloneqq \Big(-\tfrac{1}{2}\Delta + V(x)\Big)\psi_i(x) = \varepsilon_i\psi_i(x)$$

$$\rho(x,y) \coloneqq \sum_i F(\varepsilon_i)\psi_i^\star(x)\psi_i(y), \qquad \rho(x) \coloneqq \rho(x,x)$$

where $F(\varepsilon_i)$ are the single particle occupation numbers

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- $V = V[\rho] \rightsquigarrow$ self-consistent field,
- Energy: $E^{\mathrm{DFT}}[\rho] = \sum_i F(\varepsilon_i)\varepsilon_i + \ldots$

Tight Binding Model

- Discretize: $\mathcal{H}\psi_i = \varepsilon_i \psi_i$, $\mathcal{H} \in \left(\mathbb{R}^{N_\mathrm{b} \times N_\mathrm{b}}\right)^{N_\mathrm{at} \times N_\mathrm{at}}$ where

[Take $S = \mathrm{id}$ by considering Löwdin transform: $S^{-T/2}\mathcal{H}S^{1/2}$]

Orbitals

Spectrum

$$\mathcal{H}_{\ell k, ab} \coloneqq \int \phi_{\ell a}(x)\Big[-\frac{1}{2}\Delta + V(x)\Big]\phi_{kb}(x)\mathrm{d}x$$

$\{\phi_{\ell a}\}_{a=1}^{N_\mathrm{b}}$ - atom-centered localised basis functions at $\boldsymbol{r}_\ell$

More details

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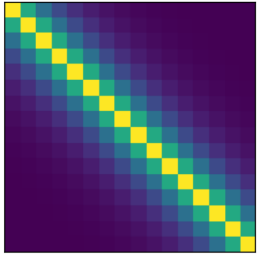
Matrix entries



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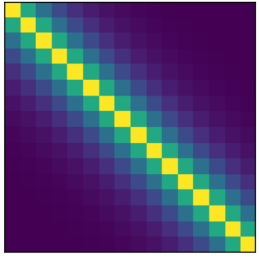

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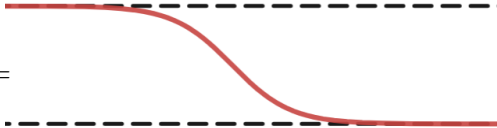
$F^\beta =$



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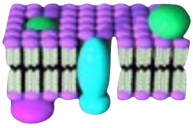

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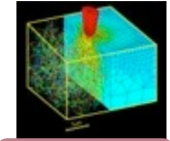
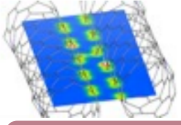


Interatomic potentials

Empirical Quantum Mechanics



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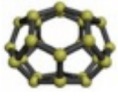
$$E^{TB}(\boldsymbol{r}) = \sum_i F(\varepsilon_i)\varepsilon_i$$



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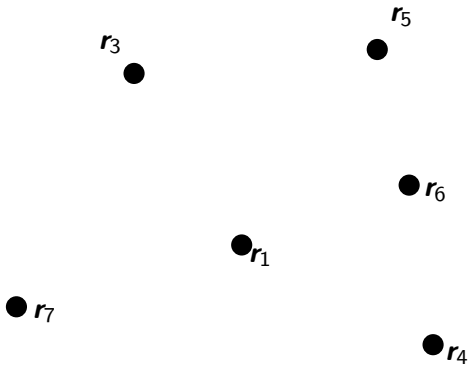
Notation

$\boldsymbol{r} = \{\boldsymbol{r}_\ell\} \subset \mathbb{R}^d$



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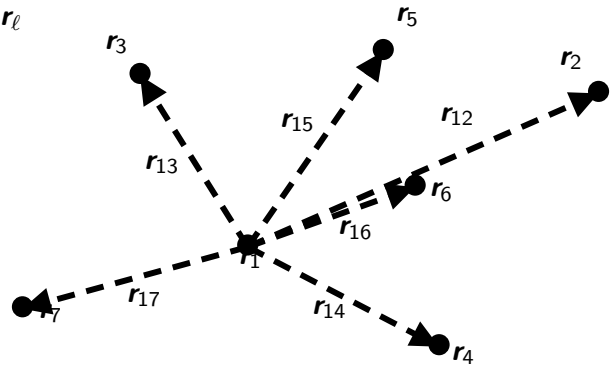

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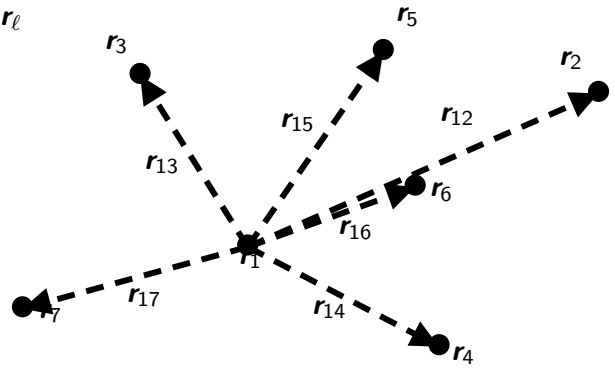

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Example: Classical interatomic potential for Si:

Stillinger–Weber:

$$E_\ell(\boldsymbol{r}) = \sum_{k\neq\ell} A\big(Br_{\ell k}^{-p} - r_{\ell k}^{-q}\big) f_{\mathrm{a}}(r_{\ell k}) + \sum_{\substack{k,m,n:\\ \ell\in\{k,m,n\}}} \lambda\big(\cos\theta_{kmn} + \tfrac{1}{3}\big)^2 f_a(r_{mk})^\gamma f_a(r_{mn})^\gamma$$

Stillinger, Weber. Phys. Rev. B 31 (1985)

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Overall, the most satisfactory parameter set thus far discovered is the following:

$$A = 7.049\,556\,277\ , \quad B = 0.602\,224\,558\,4\ ,$$
$$p = 4\ , \quad q = 0\ , \quad a = 1.80\ , \qquad (2.7)$$
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universal approximator

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Behler, Parrinello. Phys. Rev. Lett. 98 (2007)

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symmetric polynomials

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Atomic cluster expansion ACE

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Drautz. Phys. Rev. B 100 (2019)
Dusson *et al.* J. Comp. Phys. 454 (2022)

Machine Learned IPs (MLIPs)

Journal of Computational Physics 454 (2022) 110946

Atomic cluster expansion: Completeness, efficiency and stability ☆

Geneviève Dusson [a,*], Markus Bachmayr [b], Gábor Csányi [c], Ralf Drautz [d], Simon Etter [e], Cas van der Oord [c], Christoph Ortner [f]

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ACE

"All interatomic potential models make various (often ad hoc) assumptions on the PES regarding low-rank structures and locality of interactions. In general, one aims to represent a complex fully many-body PES E (exactly or approximately) as a combination of "simple" components, e.g., low-dimensional or low-rank. Here, we shall assume that E can be written in the form of a body-order expansion,

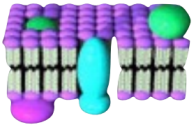
$$E\big(\{\boldsymbol{r}_1,\dots,\boldsymbol{r}_J\}\big) = \sum_{\ell=1}^{J} E_\ell\big(\{\boldsymbol{r}_{\ell k}\}_{k\neq\ell}\big)$$

$$E_\ell\big(\{\boldsymbol{r}_{\ell k}\}_{k\neq\ell}\big) = V_0 + \sum_k V_1\big(\boldsymbol{r}_{\ell k}\big) + \sum_{k_1<k_2} V_2\big(\boldsymbol{r}_{\ell k_1},\boldsymbol{r}_{\ell k_2}\big) + \cdots + \sum_{k_1<\cdots<k_N} V_N\big(\boldsymbol{r}_{\ell k_1},\dots,\boldsymbol{r}_{\ell k_n}\big), \tag{2.1}$$

with $\boldsymbol{r}_{\ell k} \coloneqq \boldsymbol{r}_k - \boldsymbol{r}_\ell$, $V_0 \in \mathbb{R}$ *and* $N \in \mathbb{N}$ *being the maximal order of interaction."*

Outline

Goal: (Qualitative) justification for the MLIP assumptions
Proof: Polynomial approximation



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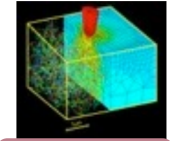

Interatomic potentials

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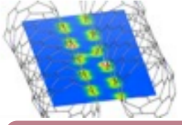

Density Functional Theory

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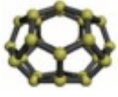

Quantum Monte Carlo

Quantum Chemistry

local decomposition into “simple” parts

Outline

Locality: Spatial Decomposition

Interatomic potentials

$$E^{IP}(\boldsymbol{r}) = \sum_{\ell} E_{\ell}^{IP}\left(\{\boldsymbol{r}_{\ell k}\}_{k \neq \ell}; \boldsymbol{\theta}\right)$$

Locality: Spatial Decomposition

- Recall:

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- Define the local observables as

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Locality: Spatial Decomposition

Interatomic potentials

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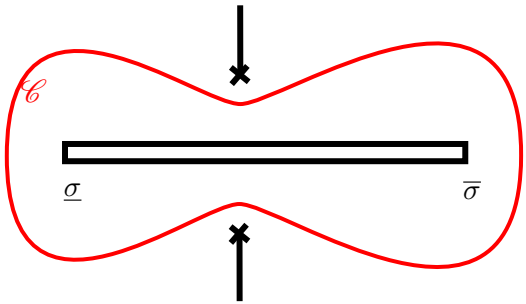

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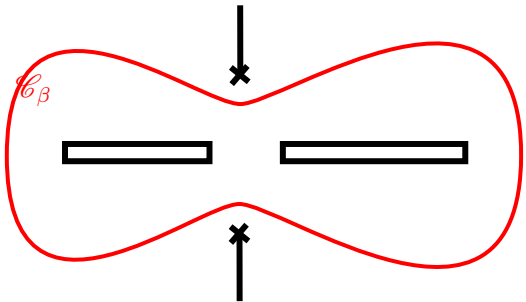

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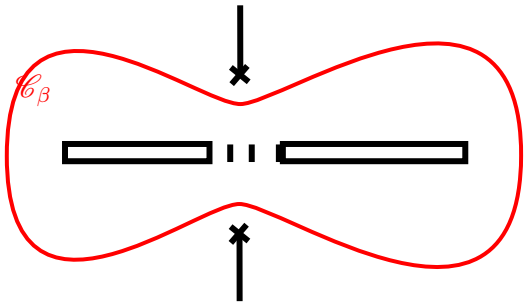

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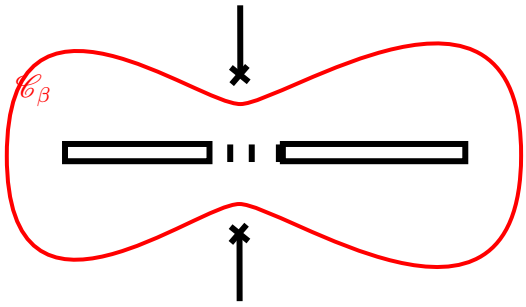

Locality: Spatial Decomposition

Tight-binding

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Numerics

$\eta > 0$ depends on:

- locality of $\mathcal{H}$,
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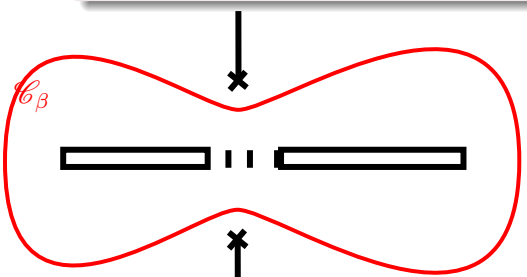

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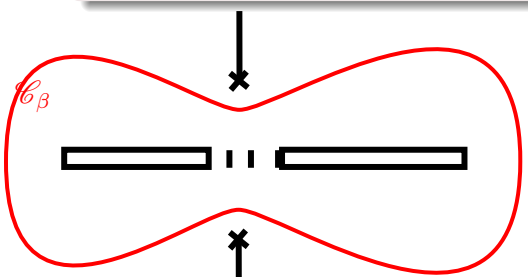

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[Chen, Ortner. Multiscale Model. Simul., 2016]
[Chen, Lu, Ortner. Arch. Rat. Mech. An., 2018]
[Ortner, JT, Chen. ESAIM: M2AN, 2020] - estimates for point defects

"Proof": Locality Estimates

Theorem:

$$\left| \frac{\partial E_\ell^{TB}(\boldsymbol{r})}{\partial \boldsymbol{r}_k} \right| \leq C e^{-\eta\, r_{\ell k}}$$

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[pictures]

"Proof": Locality Estimates

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Resolvent Estimates: Sketch for NN Hamiltonians

Suppose $\mathcal{H}_{\ell k} = 0$ for all $r_{\ell k} > 1$.
Then, $[\mathcal{H}^N]_{\ell k} = 0$ for all $r_{\ell k} > N$ and

$$\begin{aligned}\big|(z-\mathcal{H})^{-1}_{\ell k}\big| &= \min_{P_N\in\mathcal{P}_N}\big|\big[(z-\mathcal{H})^{-1} - P_N(\mathcal{H})\big]_{\ell k}\big| \\ &\leq \min_{P_N\in\mathcal{P}_N}\big\|(z-\,\cdot\,)^{-1} - P_N\big\|_{L^\infty(\sigma(\mathcal{H}))} \\ &\lesssim e^{-\gamma N} \leq e^{-\gamma r_{\ell k}}\end{aligned}$$

where $\gamma \sim \operatorname{dist}\big(z, \sigma(\mathcal{H})\big)$.

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Outline

Body-ordered approximations

Interatomic potentials

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E_ℓ - short-ranged & "simple"

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> *"In view of the fact that the Si crystal consists of atoms held in place by strong and directional bonds, it seems reasonable at first sight that the corresponding Φ could be approximated by a combination of pair and triplet potentials, V_1 and V_2."*
> — Stillinger, Weber. Phys. Rev. B 31 (1985)

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"In this so-called many-body expansion of Φ, it is usually believed that the series has a quick convergence, therefore, the higher moments may be neglected."

— Haliciogli, Pamuk, Erkoc. Phys Status Solidi B 149 (1988)

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"...the many-body potentials in general exhibit a rather slow convergence."

"It is sometimes argued that a potential expansion converges only slowly with respect to the order of the potentials and is thus impractical for use in molecular dynamics simulations."

— Drautz, Fähnle, Sanchez. J. Phys. Condens. Matter 16 (2004)

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"The convergence of the expansion is slow and, for example, for bulk metals potentials V_K up to $K \geq 15$ are required."
— Drautz. Phys. Rev. B 99 (2019)

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"Incorporating environment information leads to exponential convergence" $\implies$ replace V_n with V_{nN}

Vacuum cluster

Main idea: Polynomials are body-ordered:

$$[\mathcal{H}^n]_{\ell\ell} = \sum_{\ell_1,\ldots,\ell_{n-1}} \mathcal{H}_{\ell\ell_1}\mathcal{H}_{\ell_1\ell_2}\ldots\mathcal{H}_{\ell_{n-1}\ell}$$

["spatial correlations", "moments" $(\mathcal{H}^n)_{\ell\ell} = \int x^n \mathrm{d}D_\ell(x)$*]*

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Suppose $\varepsilon \approx \varepsilon_N$ where $\varepsilon_N \in \mathcal{P}_N$,
Then, $E_\ell^N \coloneqq \varepsilon_N(\mathcal{H})_{\ell\ell}$
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Claim:

Proof

$$\begin{aligned}&\left|E_\ell - E_\ell^N\right| \\ &\le \sup_{z\in\sigma(\mathcal{H})} |\varepsilon(z) - \varepsilon_N(z)|\end{aligned}$$

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Recall:

$$\left|E_\ell - E_\ell^N\right| \leq \|\varepsilon - \varepsilon_N\|_{L^\infty(\sigma(\mathcal{H}))}$$

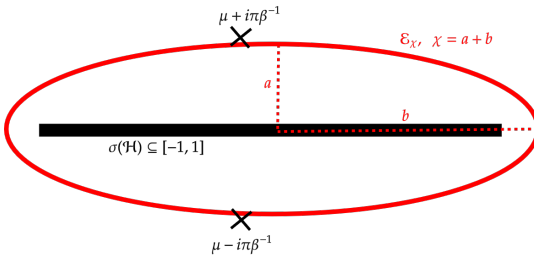
Idea #1: Upper Bounds

- Finite temperature ($T > 0$): Chebyshev projection

$$\left|E_\ell - E_\ell^N\right| \leq \frac{2\|\varepsilon\|_{L^\infty(\mathcal{E}_\chi)}}{\chi - 1}\chi^{-N}$$

where F is analytic on $\mathcal{E}_\chi$.

[Proof: Chebyshev coefficients decay exponentially depending on region of analyticity]



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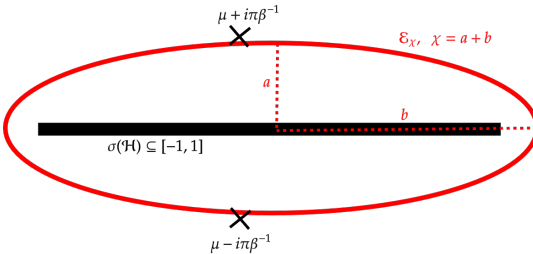

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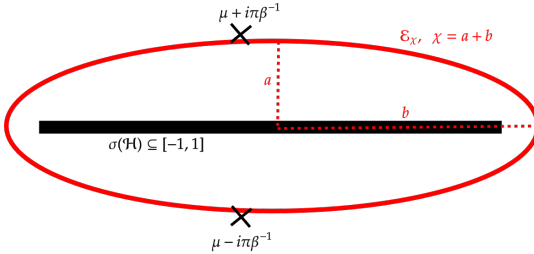

- Insulators ($g > 0$): $\exists \varepsilon_N$ s.t. [Hasson 2007]

$$\left|E_\ell - E_\ell^N\right| \le \frac{C}{\sqrt{N}}\sqrt{\frac{2-g}{2+g}}^N$$

where g is the spectral gap.

[Symmetric gap]

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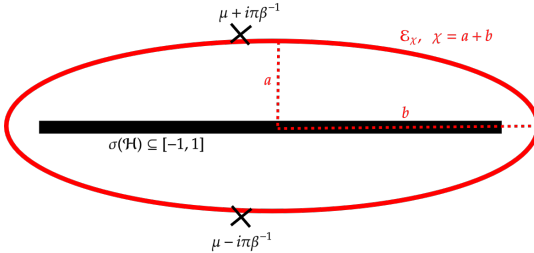
[`Proof`: Chebyshev coefficients decay exponentially depending on region of analyticity]



- Insulators ($g > 0$): $\exists \varepsilon_N$ s.t. [`Hasson 2007`]

$$\left|E_\ell - E_\ell^N\right| \le \frac{C}{\sqrt{N}}\sqrt{\frac{2-g}{2+g}}^N \sim \frac{C}{\sqrt{N}}e^{-\frac{1}{4}gN}$$

where g is the spectral gap.

[Symmetric gap]

Linear schemes: $E_\ell^N := \varepsilon_N(\mathcal{H})_{\ell\ell}$

Idea #2: Asymptotic bounds

Interpolation nodes: $X_N := \{x_j\}_{j=0}^N$

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Recall:

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Given $\Sigma \subset \mathbb{R}$, there exists an *equilibrium measure* ω_Σ such that

$$\frac{1}{N}\sum_{j=0}^{N} \delta(\,\cdot - x_j) \rightharpoonup \omega_\Sigma \quad \Longrightarrow \quad \left\|\varepsilon - \varepsilon_N\right\|_{L^\infty(\Sigma)} \lesssim e^{-\gamma_N^\star N}$$

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Example: Chebyshev nodes

$\mathrm{d}\omega_{[-1,1]}(x) = \frac{1}{\pi}\frac{1}{\sqrt{1-x^2}}\mathrm{d}x.$

Theorem (JT, Chen, Ortner (2022))

There exists a linear $\Theta_N : \mathbb{R}^N \to \mathbb{R}$ *such that*

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However,

- *Different* Θ_N *for different phases of the material*
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[Here, $\Theta_N\big(\mathcal{H}_{\ell\ell}, \dots, [\mathcal{H}^N]_{\ell\ell}\big)$ is body-ordered]

Skip ahead

Idea #3: Nonlinear schemes

- Recall, local density of states D_ℓ is a (positive) measure supported on $\sigma(\mathcal{H})$ and satisfying

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[$\mathcal{P}_N$ = polynomials degree N]

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$[\mathcal{P}_N = \text{polynomials degree } N]$

$E_\ell = \Theta_N\big(\mathcal{H}_{\ell\ell}, \ldots, [\mathcal{H}^N]_{\ell\ell}\big)$

Linear schemes:

- Chebyshev projection
  $\longrightarrow$ Kernel polynomial method[1]
- Newton–Cotes quadrature
  (equispaced nodes)
- Clenshaw–Curtis quadrature
  (Chebyshev nodes)
- General quadrature
  (with $\nu_N \rightharpoonup^\star \omega_{\sigma(\mathcal{H})}$)

Nonlinear schemes:

- Maximum entropy method[2] More
- Recursion method[3]: spectral measure corresponding to truncated tridiagonalisation of $\mathcal{H}$ More
  $\longrightarrow$ bond order potentials[4]
- Gauss quadrature More
  $\longrightarrow$ linear-scaling spectral Gauss quadrature[5]

[1] [Silver, Roeder, Voter, Kress. J. Comput. Phys. 124 (1996)]
[2] [Mead, Papanicolaou. J. Math. Phys. 25 (1984)]
[3] [Haydock, Heine, Kelly. J. Phys. C 5 (1972), 8 (1975)]
[4] [Horsfield *et al.* Phys. Rev. B 53 (1996)]
[5] [Suryanarayana *et al.* J. Mech. Phys. Solids 61 (2013)]

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where $\lim_{N\to\infty} \gamma_N = \gamma > 0$, *and* $\gamma \sim g + T$.

However,

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Numerics

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Theorem (JT, Chen, Ortner (2022))

Fix N *odd. There exist* $U \subset \mathbb{C}^N$ *and an analytic function* $\Theta_N \colon U \to \mathbb{C}$ *such that*

$$\left|E_\ell(\boldsymbol{r}) - \Theta_N\big(\mathcal{H}_{\ell\ell}, \ldots, [\mathcal{H}^N]_{\ell\ell}\big)\right| \leq Ce^{-\eta_N N}$$

where $\lim_{N\to\infty} \eta_N = \eta > 0$, *and* $\eta \sim \tilde{g} + T$.
Now,

- Θ_N *is a "universal" nonlinearity*
- *Eigenvalues in the gap* **do not** *affect the convergence rates*

However,

- Different Θ_N for different phases of the material
- Eigenvalues in the gap affect the convergence rate

$\tilde{g}$ = gap in the essential spectrum

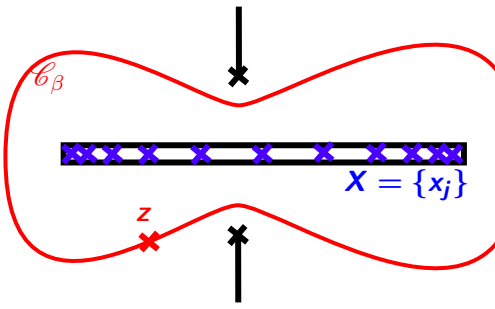
Numerics

Outline

Polynomial Approximation

Asymptotically optimal rates:

General $\Sigma \equiv \sigma(\mathcal{H})$ with $T > 0$ or $g > 0$



Polynomial Approximation

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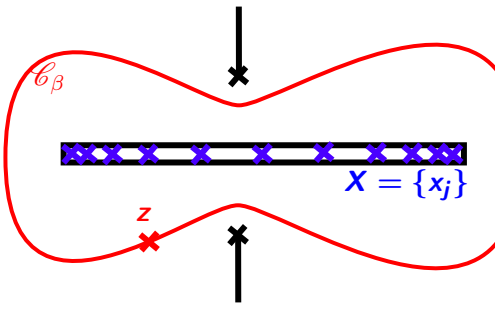
- $X = \{x_j\}_{j=0}^{N}$ – interpolation nodes



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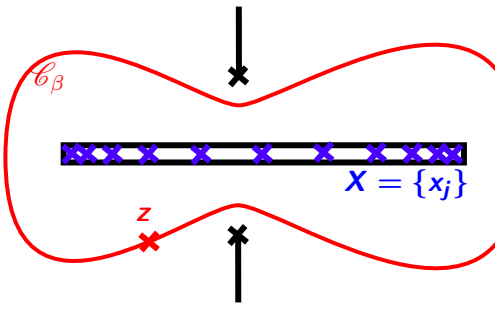

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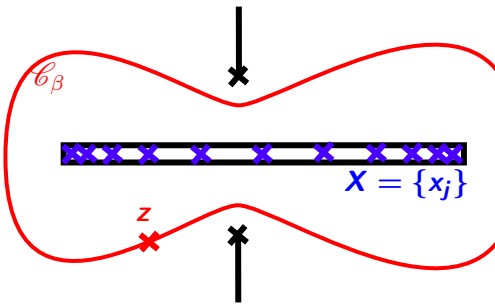
Hermite Integral formula

Let $\mathscr{C}$ contour encircling $X \cup \{x\}$,

$$\varepsilon(x) - I_X \varepsilon(x) = \oint_{\mathscr{C}} \frac{\ell(x)}{\ell(z)} \frac{\varepsilon(z)}{z - x} \frac{\mathrm{d}z}{2\pi i}$$

where $\ell(x) := \prod_{j=0}^N (x - x_j)$ is the *node polynomial*



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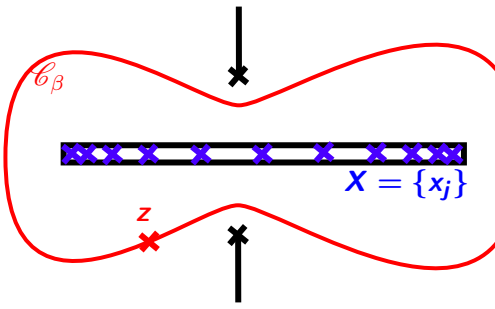


Proof:

$$\ell_j(x) = \prod_{k \neq j} \frac{x - x_k}{x_j - x_k} = \frac{\ell(x)/(x - x_j)}{\prod_{k \neq j}(x_j - x_k)} = \oint_{\mathscr{C}_j} \frac{\ell(x)/(x - z)}{\prod_{k \neq j}(z - x_k)} \frac{1}{z - x_j} \frac{\mathrm{d}z}{2\pi i} = \oint_{\mathscr{C}_j} \frac{\ell(x)}{\ell(z)} \frac{1}{x - z} \frac{\mathrm{d}z}{2\pi i}$$

Polynomial Approximation

- Hermite Integral formula $\implies$

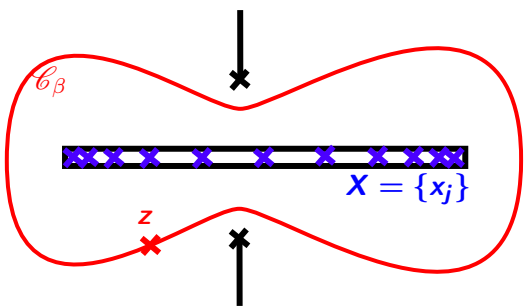
$$|\varepsilon(x) - I_X\varepsilon(x)| \leq \frac{\|\varepsilon\|_{L^\infty(\mathscr{C})}}{2\pi \mathrm{dist}\big(\sigma(\mathcal{H}), \mathscr{C}\big)} \sup_{x\in\sigma(\mathcal{H}), z\in\mathscr{C}} \left|\frac{\ell(x)}{\ell(z)}\right|$$

where $\ell(x) := \prod_{j=0}^{N}(x - x_j)$ (node polynomial),

- **Goal:** Understand the asymptotic behaviour of

$$\left|\frac{\ell(x)}{\ell(z)}\right| \qquad \text{as } N \to \infty$$

- How to choose X?



Link to Logarithmic Potential Theory

- Define $\nu_N := \frac{1}{N}\sum_{j=0}^{N}\delta_{x_j}$ and note

$$\log\left[\left|\ell(x)\right|^{\frac{1}{N}}\right] = \frac{1}{N}\sum_{j}\log\left|x-x_j\right| = \int \log|x-t|\,\mathrm{d}\nu_N(t)$$

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- body-order approx. $\longleftrightarrow$ polynomial approx.
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  $\longleftrightarrow$ behaviour of $U^\nu(x) - U^\nu(z)$

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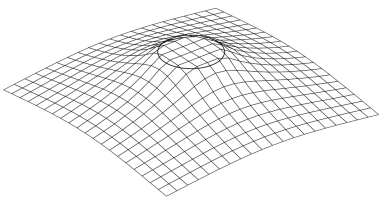

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- (Q: How to choose X to obtain this rate of approximation?)

Link to Schwarz–Christoffel mappings

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- $\exists!$ solution to this Green's function problem

$\Sigma = [-1, 1]$

Define $g_\Sigma(z) := \mathrm{Re} G_\Sigma(z)$ where

Conformal mapping problem: $G_{[-1,1]} \colon \mathbb{C}_+ \to \mathbb{C}$ s.t.

Green's function problem

Find g_Σ s.t.

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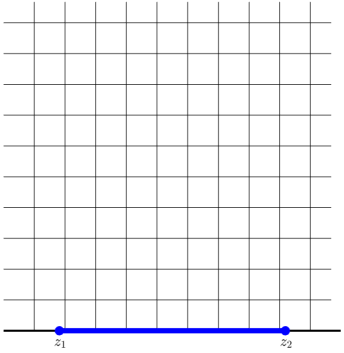
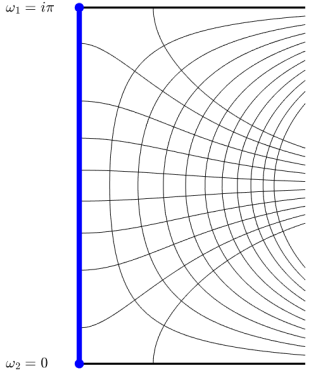


$G_{[-1,1]}$
$\longrightarrow$



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Conformal mapping problem: $G_{[-1,1]} \colon \mathbb{C}_+ \to \mathbb{C}$ s.t.

Green's function problem

Find g_Σ s.t.

- $\Delta g_\Sigma = 0$ on $\mathbb{C} \setminus \Sigma$,
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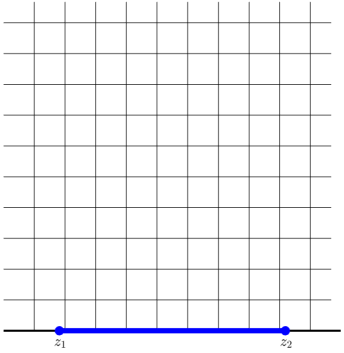

$G_{[-1,1]}$
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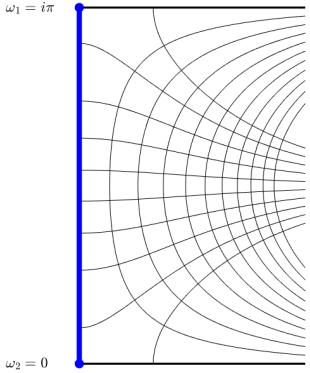

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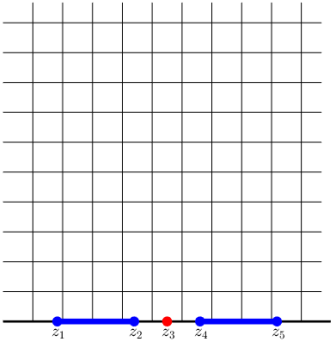

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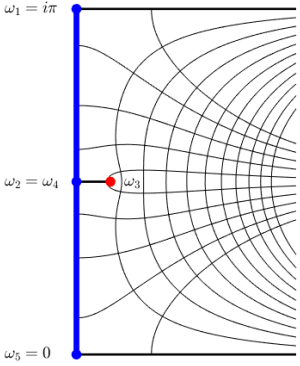

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for some $z_3 \in [a, b]$

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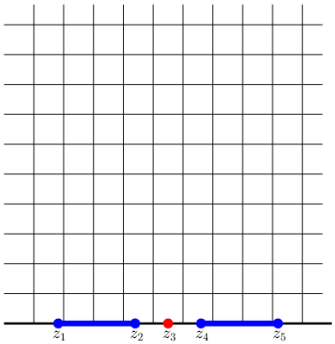

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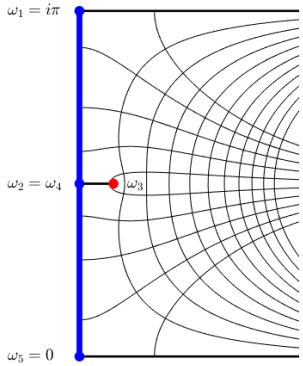

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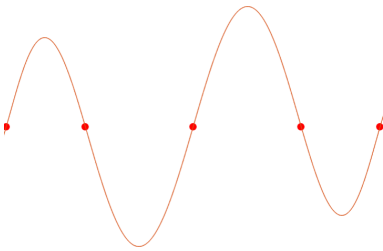

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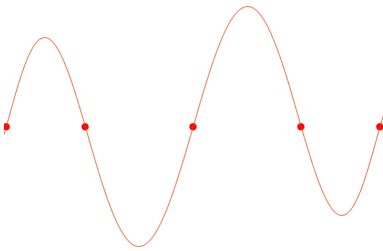

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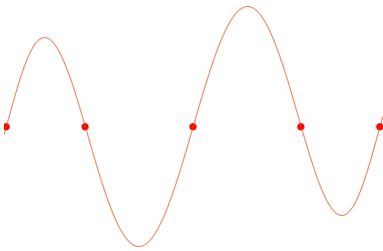

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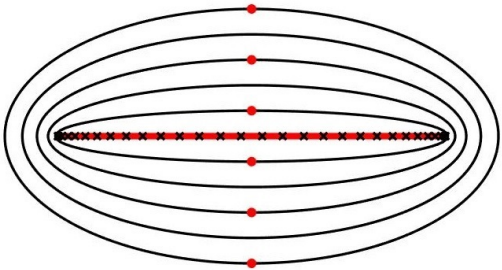

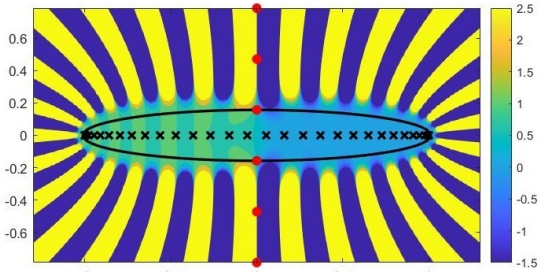

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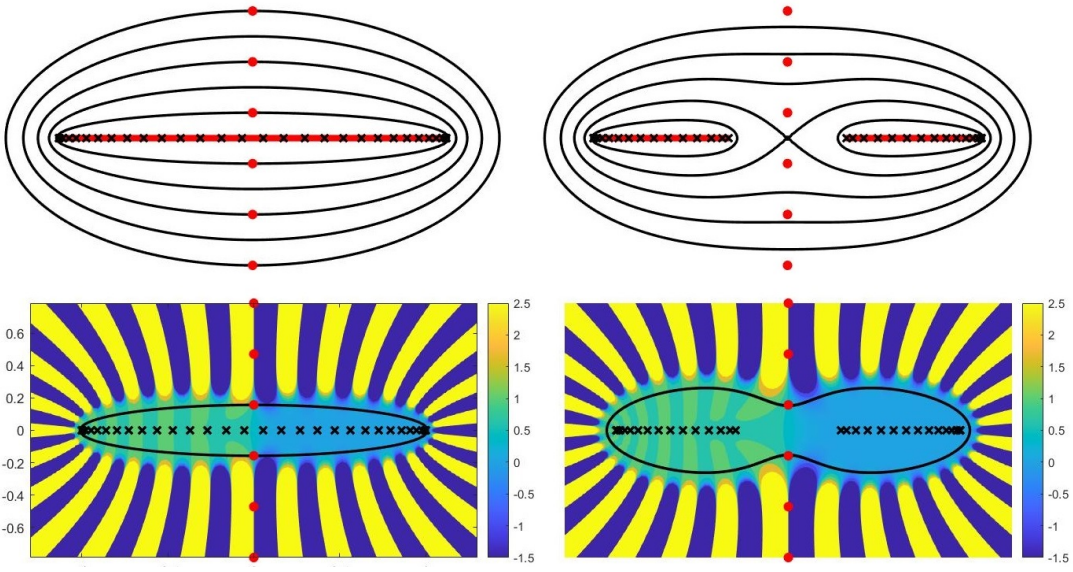

Outline

Conclusions

- $E(\boldsymbol{r}) = \sum_\ell E_\ell(\boldsymbol{r})$
  - Local pieces $\longrightarrow$ transferability
  - QM/MM schemes: size of the QM region $\sim \eta$
    [e.g. Chen, Ortner. Multiscale Model. Simul., 2016]
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- Proofs: Polynomial approximation

Arch. Rational Mech. Anal. 246 (2022) 1–60
Digital Object Identifier (DOI) https://doi.org/10.1007/s00205-022-01809-w

Body-Ordered Approximations of Atomic Properties

Jack Thomas, Huajie Chen & Christoph Ortner

Also in the paper:

- Classical vacuum cluster expansion
  [reasons for slow convergence]
- Analysis of bond-order potentials (BOP),
  [Recursion method with possibly different terminators]
- (partial) Justification for linear-scaling spectral Gauss quadrature,
  [Approximation of $\rho = F\big(\mathcal{H}[\rho]\big)$ *with* $\rho_N = F_N\big(\mathcal{H}[\rho_N]\big)$*]*
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Thank you for your attention!

What we couldn't prove (yet?):

- Forces converge in the linear schemes

$$\left| \frac{\partial E_\ell}{\partial \boldsymbol{r}_k} - \frac{\partial E_\ell^N}{\partial \boldsymbol{r}_k} \right| \lesssim e^{-\gamma r_{\ell k}} e^{-\eta N}$$

- **But**, this is a lot less obvious in the nonlinear schemes
- True if D_ℓ has *"regular n^{th} root asymptotic behaviour"*:

$$\lim_{n\to\infty} \left| p_n(z; D_\ell) \right|^{\frac{1}{n}} = e^{g_{\operatorname{supp} D_\ell}(z)}$$

  locally uniformly on $\mathbb{C} \setminus \operatorname{conv} \operatorname{supp} D_\ell$

- "Proof"

$$\left| \frac{\partial E_\ell}{\partial \boldsymbol{r}_k} - \frac{\partial E_\ell^N}{\partial \boldsymbol{r}_k} \right| \lesssim \Big[\sum_{n=0}^{\infty} \sum_{l=0}^{n} \|p_l\|^2_{L^\infty(\mathscr{C})} e^{-\eta_1 n} \Big] e^{-\eta_2 N} e^{-\gamma\, r_{\ell k}}$$

Outline

Self-consistency

- Want $\rho^\star_\ell = F\big(\mathcal{H}[\rho^\star]\big)_{\ell\ell}$,
- Approximate with $\rho_{N,\ell} = F_N\big(\mathcal{H}[\rho_N]\big)_{\ell\ell}$
  [where F_N is a body-ordered approximation of F]
- If $\rho^\star$ is *stable [linearisation is invertible]*, then there exist ρ_N such that
$$|\rho_{N,\ell} - \rho^\star_\ell| \lesssim e^{-\eta N}$$
- Can solve $\rho_{N,\ell} = F_N\big(\mathcal{H}[\rho_N]\big)_{\ell\ell}$ with the Newton iteration:
$$\rho^{i+1} = \rho^i - \big(I - DF_N(\rho^i)\big)^{-1}\big(\rho^i - F_N(\mathcal{H}[\rho^i])\big)$$

Main idea: Polynomials are body-ordered:

$$[\mathcal{H}^n]_{\ell\ell} = \sum_{\ell_1,\ldots,\ell_{n-1}} \mathcal{H}_{\ell\ell_1}\mathcal{H}_{\ell_1\ell_2}\ldots\mathcal{H}_{\ell_{n-1}\ell}$$

["spatial correlations", "moments" $(\mathcal{H}^n)_{\ell\ell} = \int x^n \mathrm{d}D_\ell(x)$]

Recall

$E_\ell = \varepsilon(\mathcal{H})_{\ell\ell} = \int \varepsilon \,\mathrm{d}D_\ell$

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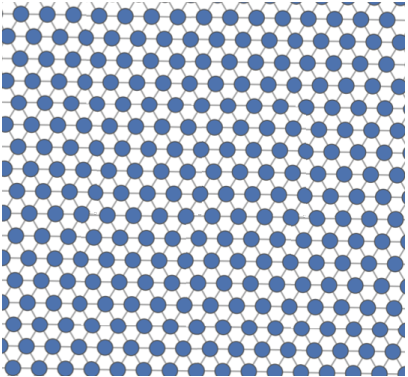
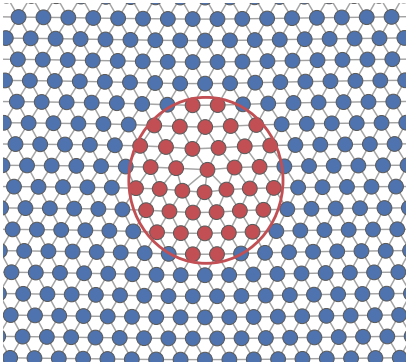
$\boldsymbol{r} =$ 

$\boldsymbol{r}^{\mathrm{def}} =$ 

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$$\{\ell\colon |\boldsymbol{r}_\ell^{\mathrm{def}}| \le R_{\mathrm{def}}\} \quad \text{finite}$$

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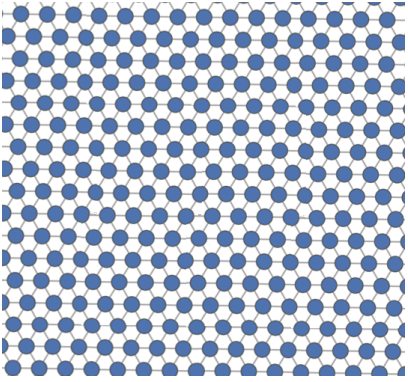

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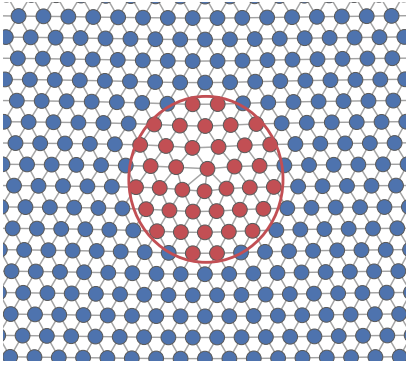
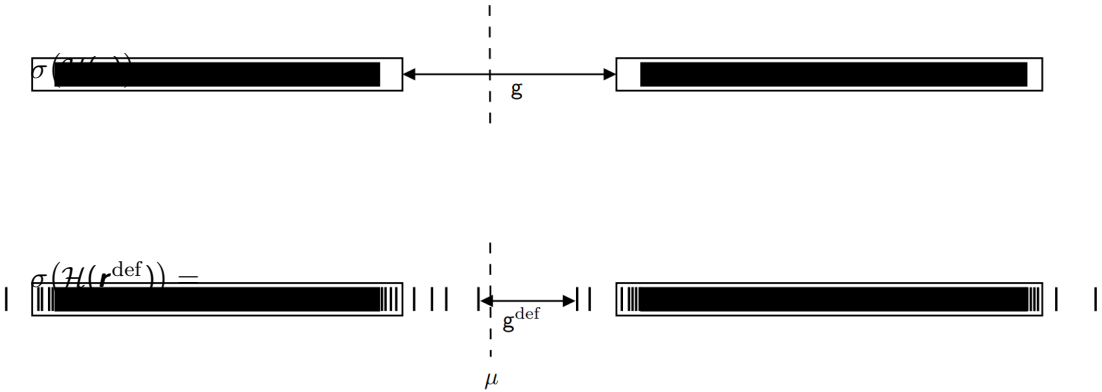


Spectrum of the Hamiltonian: Insulators



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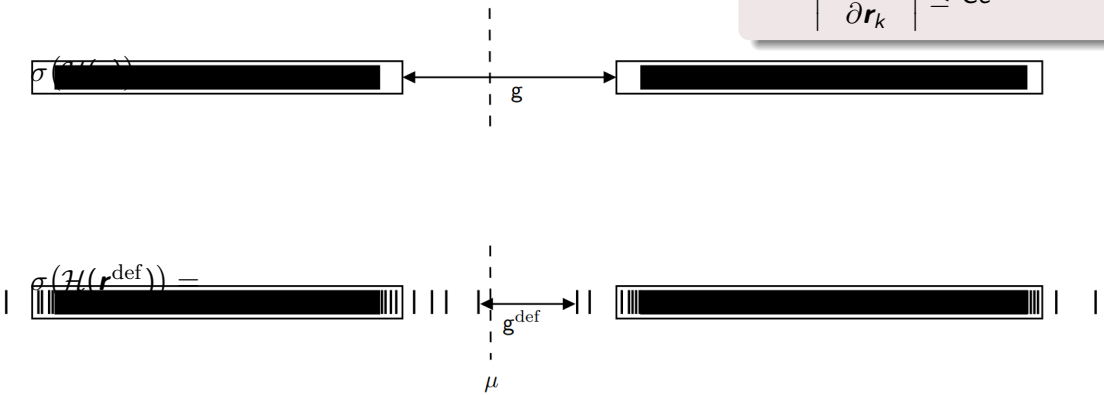

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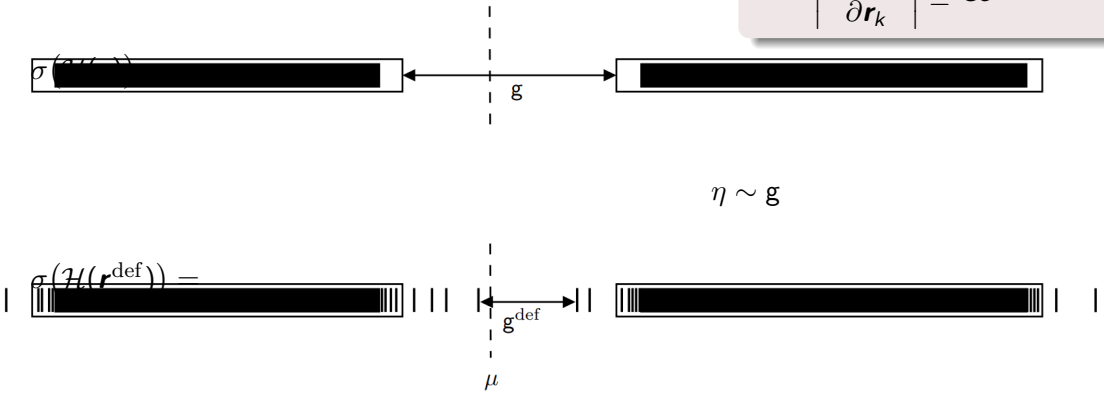

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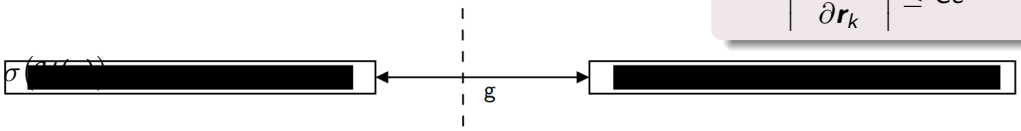
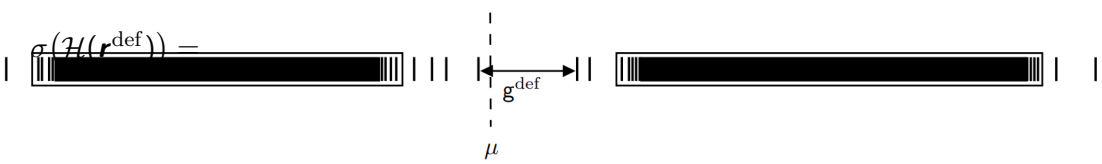


$\eta \sim \mathrm{g}$



Improved estimate:
$\eta \sim \mathrm{g} \gg \mathrm{g}^{\mathrm{def}}$

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- Schrödinger eq. $\rightsquigarrow$ *Kohn–Sham equations*

$$\mathcal{H}^{\mathrm{KS}}\psi_n := \Big(-\frac{1}{2}\Delta + V_{\mathrm{eff}}(x;\rho)\Big)\psi_n(x) = \lambda_n\psi_n(x), \qquad \rho(x) = \sum_n F(\lambda_n)\big|\psi_n(x)\big|^2$$

$F =$

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- Energy

$$E^{KS}[\rho] = \sum F(\lambda_n)\lambda_n + \ldots$$

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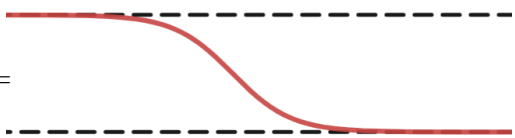
$$E^{KS}[\rho] = \sum F(\lambda_n)\lambda_n + \dots$$

$F =$ 

$F^\beta =$ 

DFT

- Schrödinger eq. $\rightsquigarrow$ *Kohn–Sham equations*

Back

$$\mathcal{H}^{\mathrm{KS}}\psi_n := \left(-\frac{1}{2}\Delta + V_{\mathrm{eff}}(x;\rho)\right)\psi_n(x) = \lambda_n\psi_n(x), \qquad \rho(x) = \sum_n F(\lambda_n)\left|\psi_n(x)\right|^2$$

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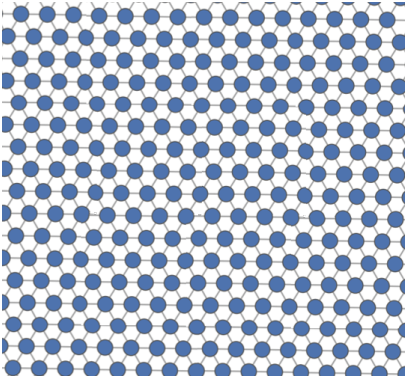
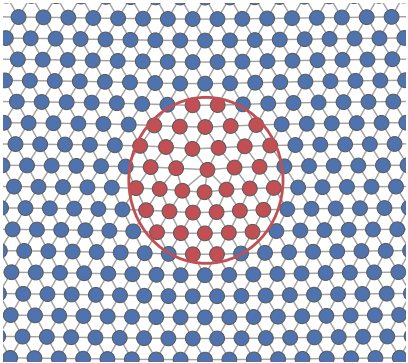
- Energy

$$E^{KS}[\rho] = \sum_n \lambda_n F(\lambda_n) - \int \rho(x) V_{\mathrm{eff}}(x;\rho) + E_{\mathrm{xc}}[\rho] + \frac{1}{2}\int\int \frac{\rho(x)\rho(y)}{|x-y|}\mathrm{d}x\mathrm{d}y - \sum_m Z_m \int \frac{\rho(x)}{|x-\boldsymbol{r}_m|}\mathrm{d}x + E_{ZZ}$$

Spectrum of the Hamiltonian

$\boldsymbol{r} =$ 

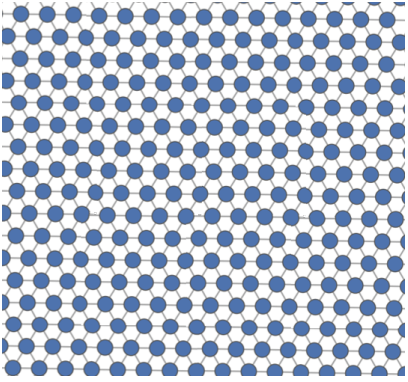
$\boldsymbol{r}^{\mathrm{def}} =$ 

Spectrum of the Hamiltonian

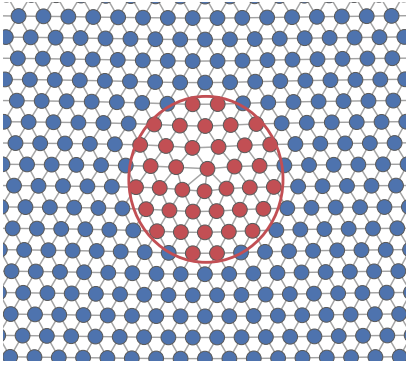
$$\{\ell\colon |\boldsymbol{r}_\ell^{\mathrm{def}}| \le R_{\mathrm{def}}\} \quad \text{finite}$$

$$\sup_{\ell\colon |\boldsymbol{r}_\ell|>R_{\mathrm{def}}} |\boldsymbol{r}_\ell^{\mathrm{def}} - \boldsymbol{r}_\ell| \le \delta$$

$\boldsymbol{r} =$

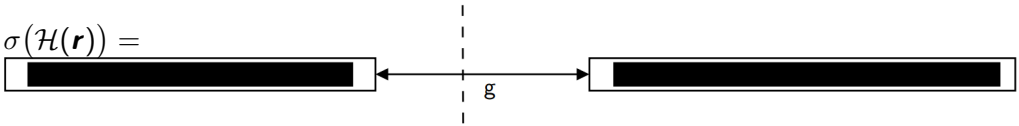


$\boldsymbol{r}^{\mathrm{def}} =$



Spectrum of the Hamiltonian: Insulators

$\sigma\big(\mathcal{H}(\boldsymbol{r})\big) =$



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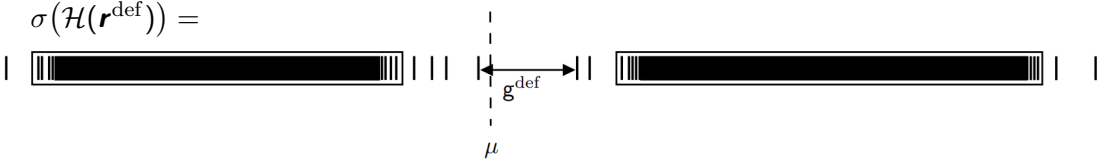
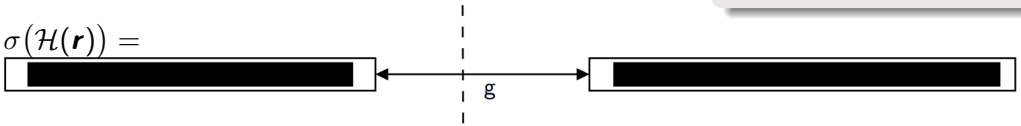


Spectrum of the Hamiltonian: Insulators

Locality:

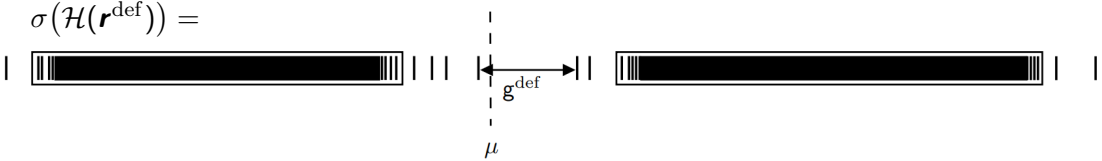
$$\left|\frac{\partial E_\ell(\boldsymbol{r})}{\partial \boldsymbol{r}_k}\right| \leq Ce^{-\eta|\boldsymbol{r}_{\ell k}|}$$

$\sigma\big(\mathcal{H}(\boldsymbol{r})\big) =$



Back

$\sigma\big(\mathcal{H}(\boldsymbol{r}^{\mathrm{def}})\big) =$



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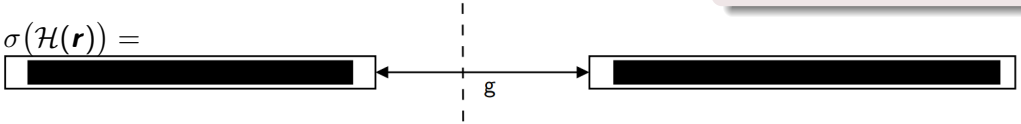
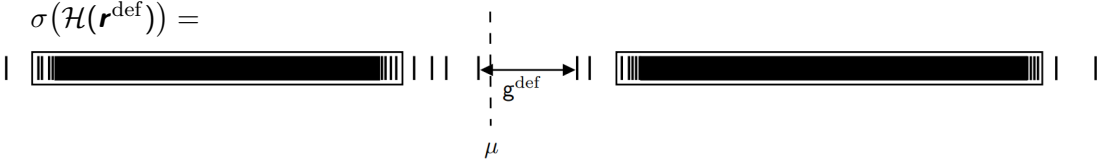


$\eta \sim \mathrm{g}$

Back

$\sigma\big(\mathcal{H}(\boldsymbol{r}^{\mathrm{def}})\big) =$



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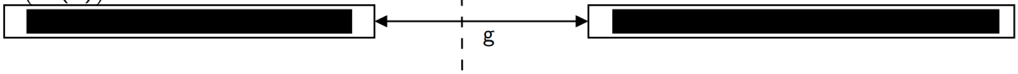
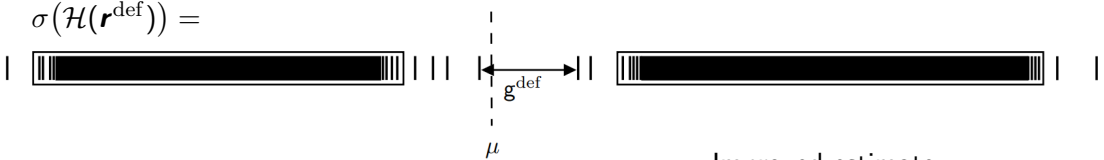


$\eta \sim \mathrm{g}$

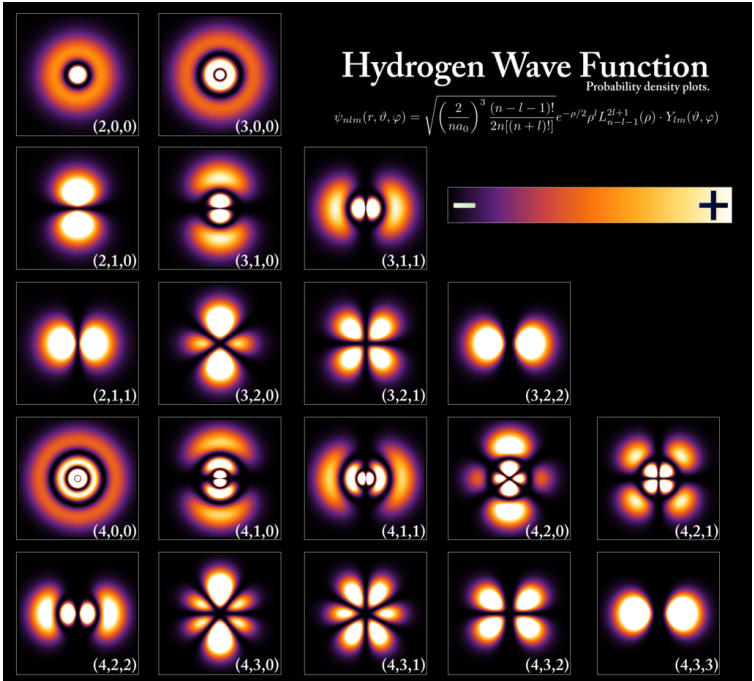
Back

$\sigma\big(\mathcal{H}(\boldsymbol{r}^{\mathrm{def}})\big) =$



Improved estimate:

$\eta \sim \mathrm{g} \gg \mathrm{g}^{\mathrm{def}}$


Hydrogen Wave Function
Probability density plots.
$\psi_{nlm}(r,\vartheta,\varphi) = \sqrt{\left(\frac{2}{na_0}\right)^3 \frac{(n-l-1)!}{2n[(n+l)!]}} e^{-\rho/2} \rho^l L_{n-l-1}^{2l+1}(\rho) \cdot Y_{lm}(\vartheta,\varphi)$
(2,0,0)
(3,0,0)
(2,1,0)
(3,1,0)
(3,1,1)
(2,1,1)
(3,2,0)
(3,2,1)
(3,2,2)
(4,0,0)
(4,1,0)
(4,1,1)
(4,2,0)
(4,2,1)
(4,2,2)
(4,3,0)
(4,3,1)
(4,3,2)
(4,3,3)

Back

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Green's Functions for Multiply Connected Domains via Conformal Mapping*

Mark Embree†
Lloyd N. Trefethen†

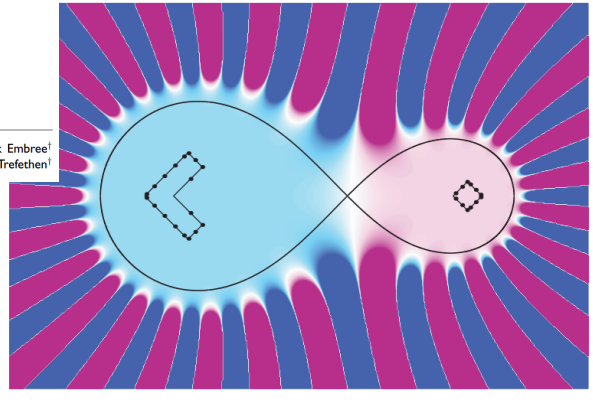

Fig. 8 *Illustration of the overconvergence phenomenon of Theorem* 2(b) *and Theorem* 4. *On the same two-polygon region as in Figure* 3, *a polynomial* $p(z)$ *is sought that approximates the values* -1 *on the hexagon and* $+1$ *on the square. For this figure,* p *is taken as the degree-*29 *near-best approximation defined by interpolation in* 30 *pre-images of roots of unity in the unit circle under the conformal map* $z = \Phi^{-1}(w)$ *(eqs.* (8) *and* (9)*); a similar plot for the exactly optimal polynomial would not look much different. The figure shows* $\mathrm{Rep}(z)$ *by a blue-red color scale together with the polygons, the interpolation points, and the figure-*8*-shaped critical level curve of the Green's function. Not just on the polygons themselves, but throughout the two lobes of the figure-*8, $\mathrm{Rep}(z)$ *comes close to the constant values* -1 *and* $+1$. *Outside, it grows very fast.*

Vacuum cluster expansion

$E\colon \bigcup_{J=0}^{\infty} \left\{ \{ \boldsymbol{r}_1, \ldots, \boldsymbol{r}_J \} \subset \mathbb{R}^3 \right\} \to \mathbb{R}$

Back

Vacuum cluster expansion

$$E\colon \bigcup_{J=0}^{\infty} \left\{ \{ \boldsymbol{r}_1, \ldots, \boldsymbol{r}_J \} \subset \mathbb{R}^3 \right\} \to \mathbb{R}$$

$$V_0 = E(\emptyset)$$

Vacuum cluster expansion

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$$V_0 = E(\emptyset)$$
$$V_1(\boldsymbol{r}_1) = E(\{\boldsymbol{r}_1\}) - E(\emptyset)$$

Back

Vacuum cluster expansion

$$E\colon \bigcup_{J=0}^{\infty} \left\{ \{\boldsymbol{r}_1, \ldots, \boldsymbol{r}_J\} \subset \mathbb{R}^3 \right\} \to \mathbb{R}$$

$$\begin{aligned} V_0 &= E(\emptyset) \\ V_1(\boldsymbol{r}_1) &= E(\{\boldsymbol{r}_1\}) - E(\emptyset) \\ V_2(\boldsymbol{r}_1, \boldsymbol{r}_2) &= E(\{\boldsymbol{r}_1, \boldsymbol{r}_2\}) - E(\{\boldsymbol{r}_1\}) - E(\{\boldsymbol{r}_2\}) + E(\emptyset) \end{aligned}$$

Back

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&\vdots \\
V_N(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_N) &= \sum_{K \subseteq \{\boldsymbol{r}_1, \ldots, \boldsymbol{r}_N\}} (-1)^{N-|K|} E(K)
\end{aligned}$$

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Then,

$$E(\{\boldsymbol{r}_1, \ldots, \boldsymbol{r}_J\}) \approx \sum_{n=0}^{N} \sum_{j_1 < \cdots < j_n} V_n(\boldsymbol{r}_{j_1}, \ldots, \boldsymbol{r}_{j_n})$$

Exact for $N = J$.

Back

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Exact for $N = J$.

Convergence? Rate of convergence? Not clear!

"An intuitive explanation for this slow convergence is that we are building an interaction law for a condensed or possibly even crystalline phase material from clusters in vacuum where the bonding chemistry is significantly different."

Back

Vacuum cluster expansion

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Exact for $N = J$.

Convergence? Rate of convergence? Not clear!

Instead:

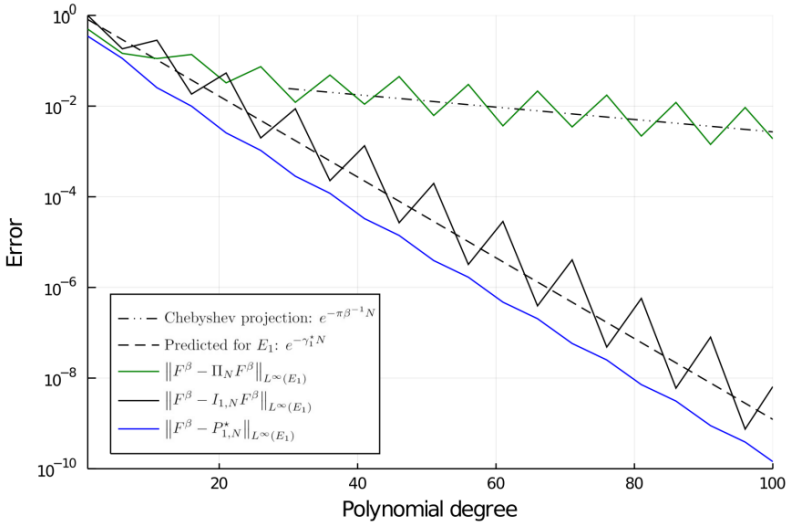
Replace V_n with V_{nN}

"An intuitive explanation for this slow convergence is that we are building an interaction law for a condensed or possibly even crystalline phase material from clusters in vacuum where the bonding chemistry is significantly different."

Back

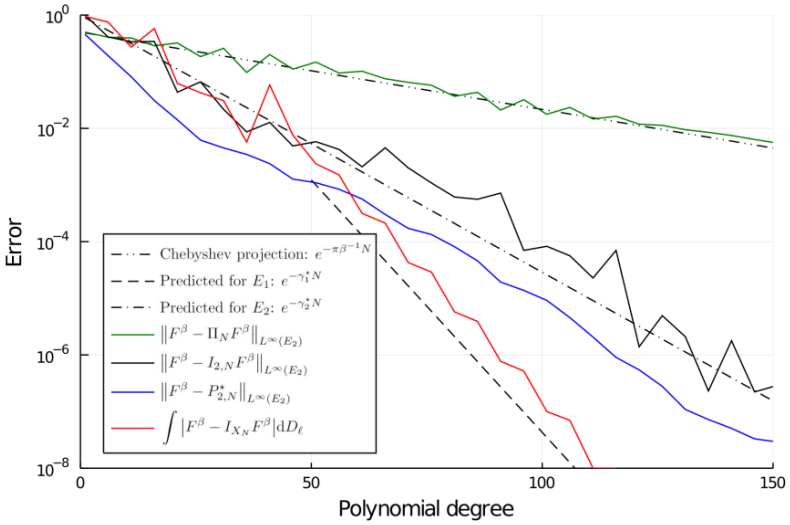
Numerical experiments: "defect-free"

- Approximation domain $E_1 = [-1, -0.2] \cup [0.2, 1]$



Numerical experiments: with defect

- Approximation domain $E_2 = E_1 \cup [-0.06, -0.03]$



Back

Maximum entropy method

- Fix $[a, b] \supset \sigma(\mathcal{H})$, maximise

$$S(P) \coloneqq -\int_a^b \big[P(x)\log P(x) - P(x)\big]\,\mathrm{d}x + \sum_{n=0}^{N} \lambda_n \left(\int_a^b x^n P(x)\mathrm{d}x - [\mathcal{H}^n]_{\ell\ell} \right)$$

- Leads to

$$P_N(x) = e^{-\sum_{n=0}^{N} \lambda_n x^n} \qquad \text{s.t. first } N \text{ moments}$$

- Moreover, if $\{(\mathcal{H}^n)_{\ell\ell}\}$ is completely monotone, then $\exists! P$.

Back

Nonlinear schemes: Recursion method

- Let $\{p_n\}$ orthogonal polynomials with respect to D_ℓ:

$$b_{n+1}p_{n+1}(x) = (x - a_n)p_n(x) - b_n p_{n-1}(x) \qquad \text{[Lanczos recursion]}$$

define

$$T_N := \begin{pmatrix} a_0 & b_1 & & \\ b_1 & a_1 & \ddots & \\ & \ddots & \ddots & b_N \\ & & b_N & a_N \end{pmatrix} = \Big(\int p_i(x) x p_j(x) \mathrm{d}D_\ell(x) \Big)_{0 \le i,j \le N},$$

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- $[\mathcal{H}^n]_{\ell\ell} = [(T_N)^n]_{00}$ for all $n \le 2N + 1$,

Back

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$$\big| E_\ell(\boldsymbol{r}) - E_\ell^N(\boldsymbol{r}) \big| \le 2 \inf_{\varepsilon_{2N+1} \in \mathcal{P}_{2N+1}} \big\| \varepsilon - \varepsilon_{2N+1} \big\|_{L^\infty(\sigma(\mathcal{H}) \cup \mathrm{supp}(D_\ell^N))}$$

Back

If $\mathrm{supp}(D_\ell) \cap [a,b] = \emptyset$, then $|\mathrm{supp}(D_\ell^N) \cap [a,b]| \leq 1$

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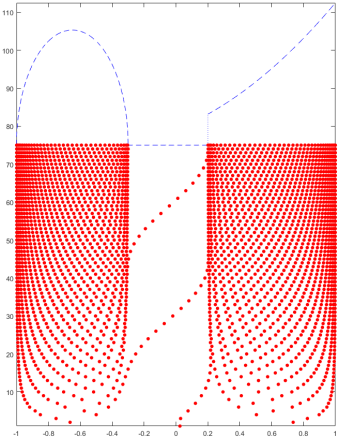

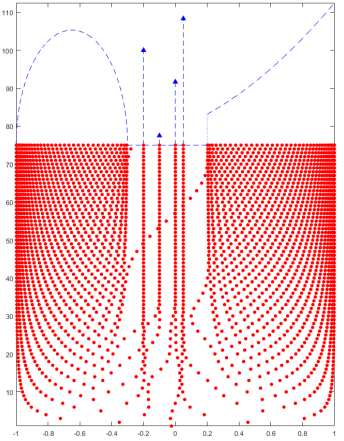

Back

Nonlinear schemes: Gauss quadrature

- Let $\{p_n\}$ orthogonal polynomials with respect to D_ℓ,
- Interpolate in $X \coloneqq \{\text{zeros of } p_{N+1}\}$,

Nonlinear schemes: Gauss quadrature

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$\mathrm{supp}(D_\ell^N)$ "nice enough"

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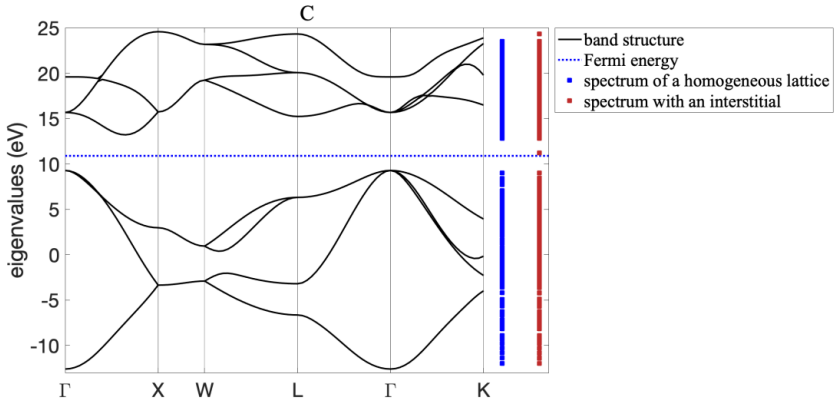
$\mathrm{supp}(D_\ell^N)$ "nice enough"

- Can show that $E_\ell^N = \Theta\left(\mathcal{H}_{\ell\ell}, \ldots, (\mathcal{H}^{2N+1})_{\ell\ell}\right)$ where $\Theta\colon \mathbb{C}^{2N+1} \to \mathbb{C}$ is analytic in open neighbourhoods of "admissible moment sequences"

Back

Numerical Experiments



[Ortner, JT, Chen. ESAIM: M2AN, 2020]

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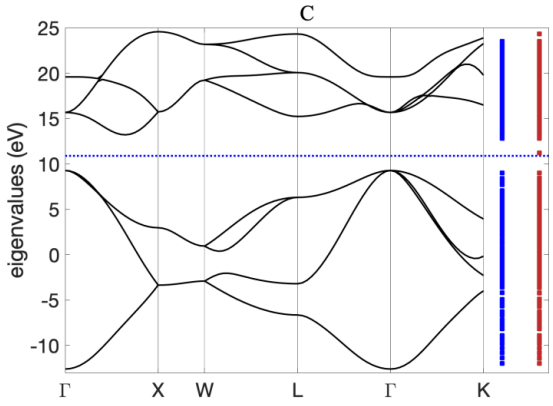

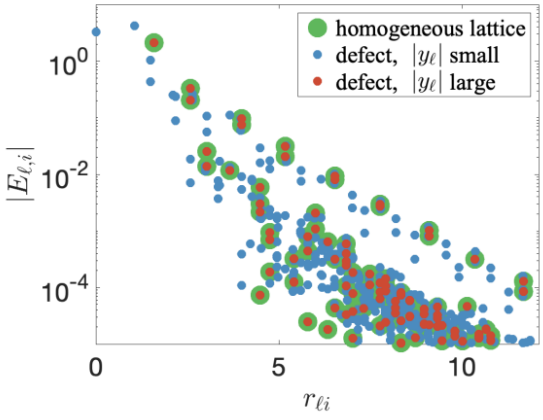

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(a) Decay of site energy derivatives.

Atomic Cluster Expansion (ACE)

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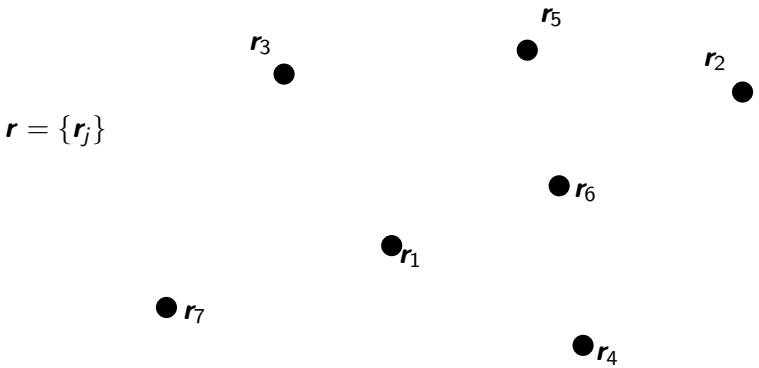

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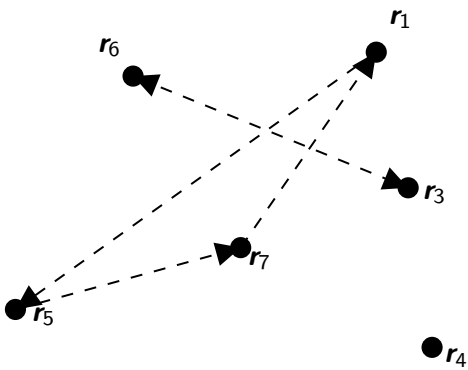

- Permutations

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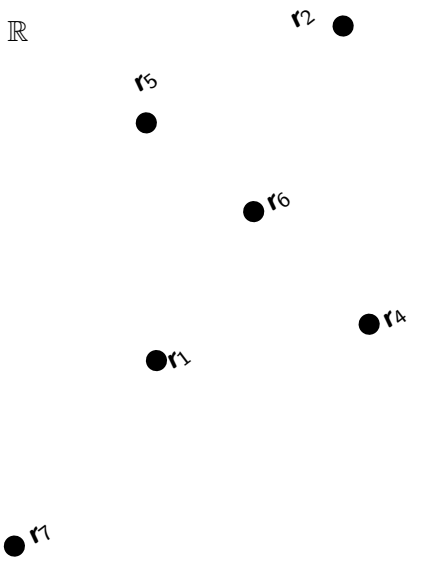

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— Bachmayr *et al.* J. Comp. Phys. 454 (2022)

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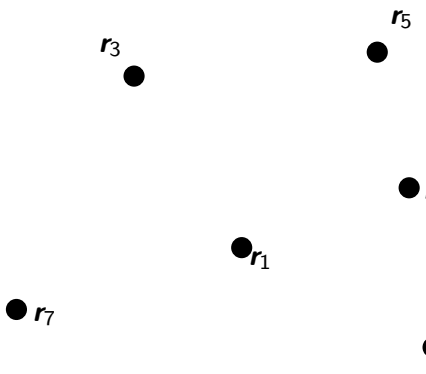

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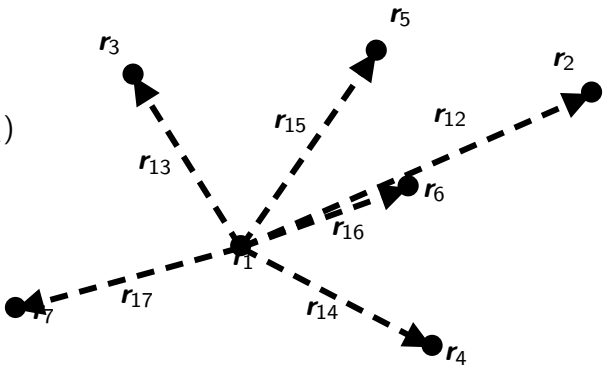

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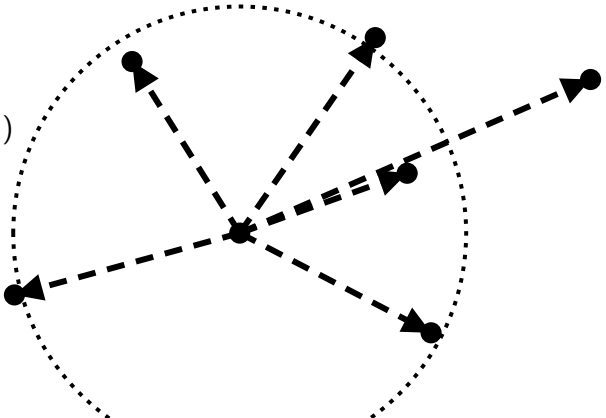

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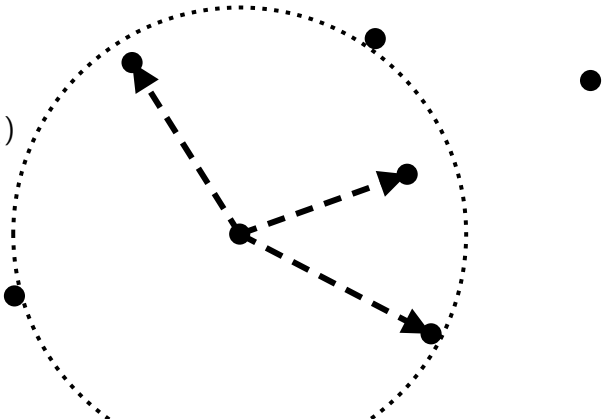

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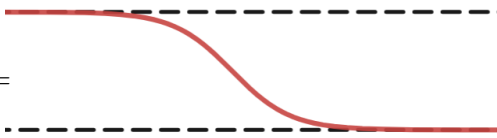

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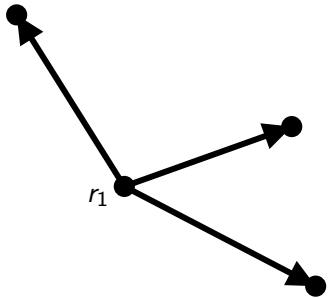

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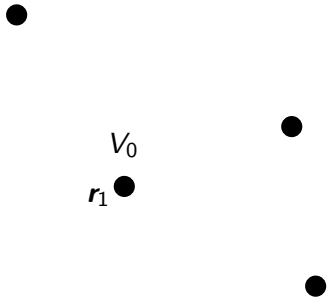

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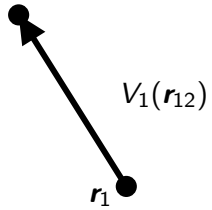
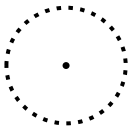


$E_1 =$ V_0 $+$

$=$



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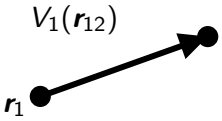

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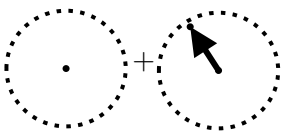
$$=$$ 

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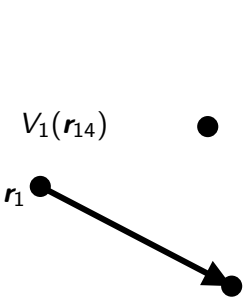

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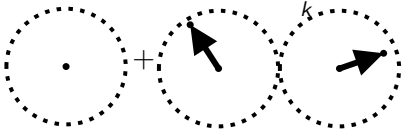

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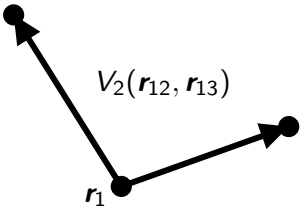

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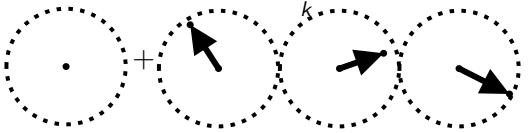

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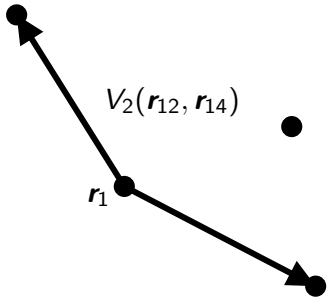

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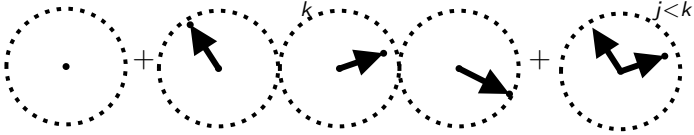

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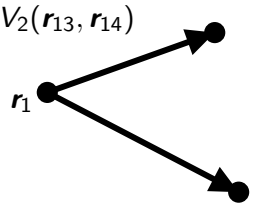

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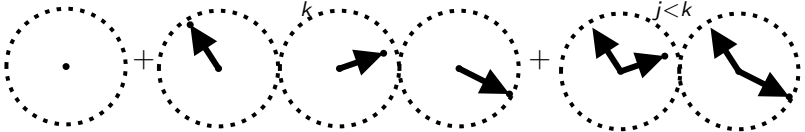

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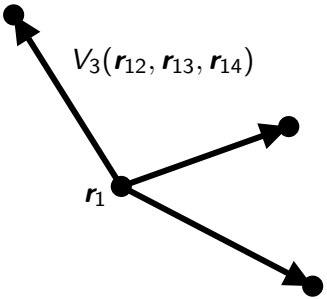
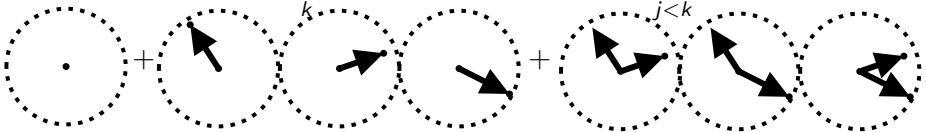


$$E_1 = V_0 + \sum_k V_1(\boldsymbol{r}_{1k}) + \sum_{j<k} V_2(\boldsymbol{r}_{1j}, \boldsymbol{r}_{1,k}) +$$

$$=$$



Atomic Cluster Expansion

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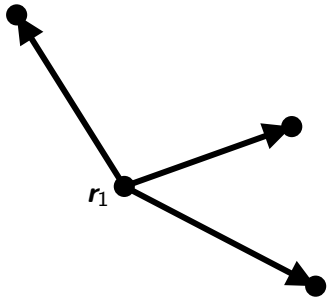

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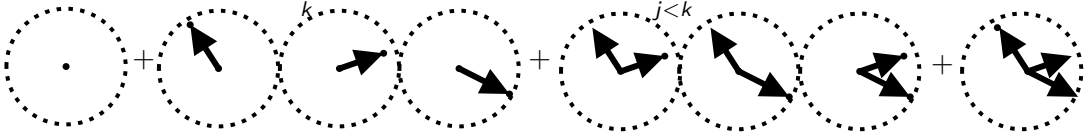

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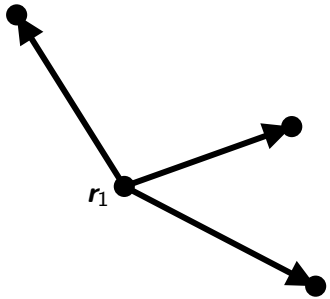

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Approximate $\boldsymbol{R} = (\boldsymbol{r}_1, \dots, \boldsymbol{r}_N) \mapsto V_N(\boldsymbol{R})$ where

- $V_N(\boldsymbol{R}) = 0$ if $\max |\boldsymbol{r}_j| \geq r_{\text{cut}}$,
- $V_N(Q\boldsymbol{R}) = V_N(\boldsymbol{R})$ where $Q\boldsymbol{R} = (Q\boldsymbol{r}_j)_{j=1}^N$, $Q \in O(3)$,
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Computationally efficient? For $J \gg \mathcal{N}$, naively scales like $\binom{J}{\mathcal{N}} \sim \frac{J^{\mathcal{N}}}{\mathcal{N}!}$

ACE: Approximate $V_N(\boldsymbol{R})$ where $\boldsymbol{R} = (\boldsymbol{r}_1, \ldots, \boldsymbol{r}_N) \in \mathbb{R}^{3N}$

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- Restrict V_N to $\{\boldsymbol{r} \in \mathbb{R}^3 \colon |\boldsymbol{r}| > r_0\}^N$
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ACE: Trick

(Naive) Cost: compute basis $N!$, evaluate following $\binom{J}{N}$

$$\sum_{j_1<\cdots<j_N} \widetilde{V}_N(\boldsymbol{r}_{j_1},\ldots,\boldsymbol{r}_{j_N}) = \sum_{\boldsymbol{nl}i} \widetilde{c}_{\boldsymbol{nl}i} \sum_{j_1<\cdots<j_N} \mathcal{B}_{\boldsymbol{nl}i}(\boldsymbol{r}_{j_1},\ldots,\boldsymbol{r}_{j_N})$$

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$$= \sum_{\boldsymbol{m}} \boldsymbol{C}_{\boldsymbol{m}}^{(\boldsymbol{nl}i)} \sum_{j_1,\ldots,j_N} \prod_{\alpha=1}^{N} \phi_{n_\alpha l_\alpha m_\alpha}\left(\boldsymbol{r}_{j_\alpha}\right)$$

$$= \boxed{\sum_{\boldsymbol{m}} \boldsymbol{C}_{\boldsymbol{m}}^{(\boldsymbol{nl}i)} \prod_{\alpha=1}^{N} \sum_{j=1}^{J} \phi_{n_\alpha l_\alpha m_\alpha}(\boldsymbol{r}_j)}$$

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V

ACE: Trick

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ACE = expansion in terms of the basis $\bigcup_{N=0}^{\infty}\{B_{\boldsymbol{nl}i} : \boldsymbol{n},\boldsymbol{l}\in\mathbb{N}^N,\ldots\}$

$\Sigma = [-1, a] \cup [b, 1]$

Define $g_\Sigma(z) := \mathrm{Re} G_\Sigma(z)$ where

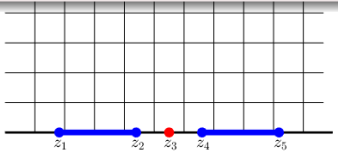
Green's function problem

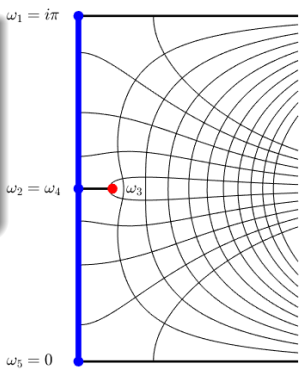
Find g_Σ s.t.

- $\Delta g_\Sigma = 0$ on $\mathbb{C} \setminus \Sigma$,
- $g_\Sigma(z) \sim \log|z|$ as $z \to \infty$,
- $g_\Sigma = 0$ on Σ.

$z_3 \in [a, b]$ s.t. $G_\Sigma(a) = G_\Sigma(b)$

$$z_3 = \frac{\displaystyle\int_a^b \frac{\zeta}{\sqrt{\zeta+1}\sqrt{\zeta-a}\sqrt{\zeta-b}\sqrt{\zeta-1}}\mathrm{d}\zeta}{\displaystyle\int_a^b \frac{1}{\sqrt{\zeta+1}\sqrt{\zeta-a}\sqrt{\zeta-b}\sqrt{\zeta-1}}\mathrm{d}\zeta}$$





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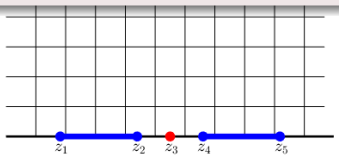
$$G_{[-1,a]\cup[b,1]}(z) = \int_1^z \frac{\zeta - z_3}{\sqrt{\zeta+1}\sqrt{\zeta-a}\sqrt{\zeta-b}\sqrt{\zeta-1}} \mathrm{d}\zeta,$$

for some $z_3 \in [a, b]$

$z_3 \in [a, b]$ s.t. $G_\Sigma(a) = G_\Sigma(b)$

$$z_3 = \frac{\displaystyle\int_a^b \frac{\zeta}{\sqrt{\zeta+1}\sqrt{\zeta-a}\sqrt{\zeta-b}\sqrt{\zeta-1}} \mathrm{d}\zeta}{\displaystyle\int_a^b \frac{1}{\sqrt{\zeta+1}\sqrt{\zeta-a}\sqrt{\zeta-b}\sqrt{\zeta-1}} \mathrm{d}\zeta}$$



Green's function problem

Find g_Σ s.t.

- $\Delta g_\Sigma = 0$ on $\mathbb{C} \setminus \Sigma$,
- $g_\Sigma(z) \sim \log|z|$ as $z \to \infty$,
- $g_\Sigma = 0$ on Σ.