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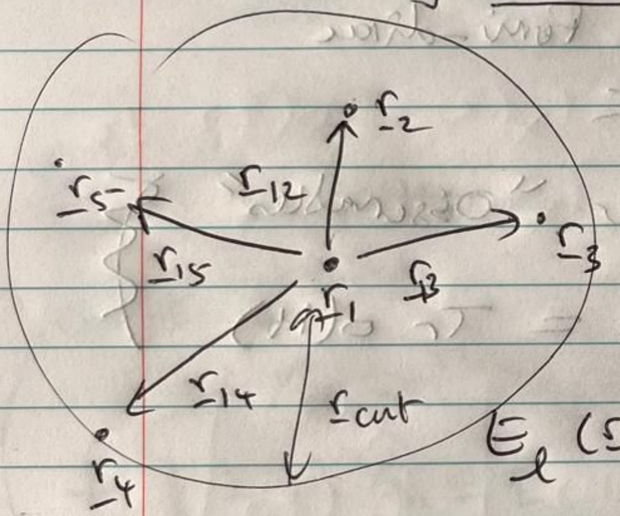
Body-ordered Approximations

ARMA 246 (2022)
JT, Chen, Ortner

* Justify interatomic potentials



$$E(r) = \sum_\ell E_\ell(r)$$

Notation $r \subset \mathbb{R}^d$

$r_{\ell k} = r_k - r_\ell$, $r_{\ell k} = |r_{\ell k}|$

$$E_\ell(r) = E_\ell(\{r_{\ell k}\}_{r_{\ell k} < r_{cut}})$$

LOCALITY "short-ranged"

E_ℓ "simple"

Examples EAM, SW

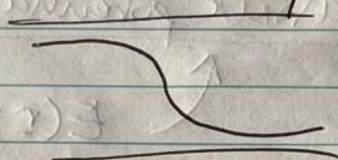
linear 3-body

non-linear
body-order 2
(correlation order 1)

start from tight binding

$$|H(r)_{lk}| \lesssim e^{-\gamma_0 r_{lk}}$$

Band energy : $E = \sum_i f(\varepsilon_i)\, \varepsilon_i = \mathrm{Tr}\, H f^\beta(H)$



Fermi-dirac

More generally, we consider "observables"

$$O = \sum_i o(\varepsilon_i) = \mathrm{Tr}\, o(H)$$

LOCALITY

$$O = \mathrm{Tr}\, o(H) = \sum_l o(H)_{ll}$$

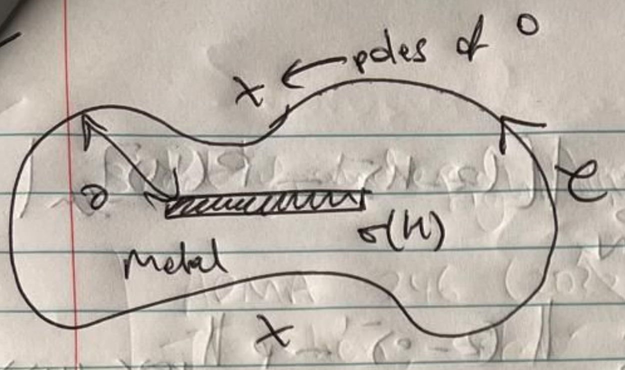
$$O_l := o(H)_{ll}$$

$$= \oint_{\mathcal{C}} o(z)\, (z-H)^{-1}_{ll} \frac{dz}{2\pi i}$$

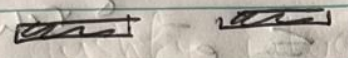
"local observables"

e.g. electron density $\rho_l = f^\beta(H)_{ll}$

grand potential $G(x) = \frac{2}{\beta} \log\left(1 - f^\beta\right)(x)$



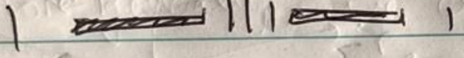
e.g. F^β has poles @ $\mu + i\pi\beta^{-1}(2\mathbb{Z}+1)$



Insulator

Thm 1 (Locality)

$$\left|\frac{\partial O_\ell}{\partial r_k}\right| \lesssim e^{-\gamma r_{\ell k}}$$



Point defect

Proof Combes–Thomas (not me)

γ – depends on γ_0, analyticity of O, $\sigma(H)$

$\Rightarrow \gamma = c\min(1, d)$

Combes–Thomas

Proof $B_{\ell k} = e^{\gamma r_{\ell k_0}} A_{\ell k} e^{-\gamma r_{k k_0}}$

$+ \ \|I - A^{-1}B\| \le \frac{1}{2}$

Fun proof

(NN interactions) or banded

If $H_{\ell k} = 0$ for $r_{\ell k} > 1$

Then $(H^N)_{\ell k} = 0$ for $r_{\ell k} > N$

$$\| \quad \sum_{\ell_1,\dots,\ell_{N-1}} H_{\ell\ell_1} H_{\ell_1\ell_2} \cdots H_{\ell_{N-1}k}$$

So for $r_{lk} > N$

$$|(z-H)^{-1}_{lk}| = \min_{p \in \mathcal{P}_N} \left|\left[(z-H)^{-1} - p(H)\right]_{lk}\right|$$

$$\le \min_{p \in \mathcal{P}_N} \|(z-\cdot)^{-1} - p\|_{L^\infty(\sigma(H))}$$

$$\lesssim e^{-\gamma N} \le e^{-\gamma r_{lk}}$$

where $\gamma \sim \mathrm{dist}(z, \sigma(H))$, use Cauchy integral □

Therefore

$$O_l(\Sigma) = O_l(\{r_{lk}\}_{k:\, r_{lk} < r_{cut}}) + O(e^{-\gamma r_{cut}})$$

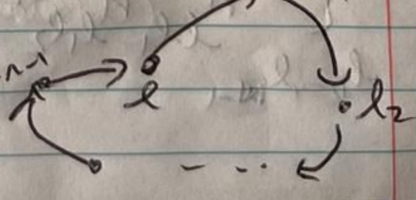
In practice O_l still high-dimensional!

$\rightsquigarrow$ body ordered expansion

$$E_l \approx V_0 + \sum_{k \neq l} V_1(r_{lk}) + \sum_{k_1, k_2 \neq l} V_2(r_{lk_1}, r_{lk_2}) + \dots + \sum_{k_1, \dots, k_N} V_N(r_{lk_1}, \dots, r_{lk_N})$$

<u>Idea</u> Polynomials are body-ordered!

(look back at $(H^n)_{lk}$)



Approximate $O_\ell = O(H)_{\ell\ell}$

using $(H^n)_{\ell\ell}$ for $n = 0, \dots, N$

Idea #1 Approximate O_ℓ with

$$O_\ell^N := o^N(H)_{\ell\ell} \text{ for some polynomial } o^N$$

Error

$$|O_\ell - O_\ell^N| = |[o(H) - o^N(H)]_{\ell\ell}|$$

$$\le \| o(H) - o^N(H) \|_{\ell^2 \to \ell^2}$$

$$= \sup_{z \in \sigma(H)} |o(z) - o^N(z)|$$

Julia $o = f^\beta(\cdot - \mu)$

$$o^N := I_{X_N} o$$

interpolation in points X_N

See back

$$\ell_X(z) = \prod_{x \in X} (z - x)$$

$$I_{X_N} o(z) = \sum_{x \in X_N} o(x) \underbrace{\prod_{y \in X_N \setminus \{x\}} \frac{z - y}{x - y}}_{x \mapsto 1,\ y \neq x \mapsto 0}$$

$o^N(H)_{\ell\ell}$ linear function of $(H^n)_{\ell\ell}$

Linear schemes

$$O_\ell = O(H)_{\ell\ell} \approx o^N(H)_{\ell\ell}$$

$$\| \qquad\qquad \|$$

$$\int o(x)\, \underbrace{dD_\ell(x)}_{\text{spectral measure}} \qquad \int o^N(x)\, dD_\ell(x)$$

$$\|$$

$$\int o(x)\, dD_\ell^N(x)$$

$$\sum_{x \in X_N} \boxed{\ell_x(H)_{\ell\ell}}\, \delta(\cdot - x)$$

$$\ell_x(z) := \prod_{y \in X_N \setminus \{x\}} \frac{z-y}{x-y}$$

$$\ell_x(y) = \delta_{xy} \text{ for } x, y \in X_N$$

"Method of moments"

More generally choose any D_ℓ^N s.t.

$$(H^n)_{\ell\ell} = \int x^n \, dD_\ell^N \qquad n = 0, \dots, N$$

Define $O_\ell^N := \int o(x)\, dD_\ell^N(x)$

~~[illegible]~~

Error estimates

$$|O_\ell - O_\ell^N| = \left| \int o(x) \, d(D_\ell - D_\ell^N)(x) \right|$$

$$= \min_{p \in P_N} \left| \int (o(x) - p(x)) \, d(D_\ell - D_\ell^N)(x) \right|$$

$$\leq \min_{p \in P_N} \| o - p \|_\infty \underbrace{\| D_\ell - D_\ell^N \|_\infty}_{\text{operator norm on a fn space } (S, \|\cdot\|_\infty)}$$

w/ ~~[illegible]~~

e.g.

S – functions analytic in (nbhd of $\sigma(H)) \supseteq \mathcal{C}$

$\|\cdot\|_\infty := \frac{\operatorname{len} \mathcal{C}}{2\pi} \| o \|_{L^\infty(\mathcal{C})}$

e.g. 2

$S = L^\infty(\operatorname{supp}(D_\ell - D_\ell^N))$

$\|\cdot\|_\infty = \|\cdot\|_{TV}$

* Analyticity of o

* Spectral pollution $\operatorname{supp} D_\ell^N \not\subseteq \sigma(H)$ in general

* regularity of D_ℓ^N

Polynomial Interpolation on X_N

$$\| D_\ell^N \|_{TV} = \sup_{\substack{\|g\|_{L^\infty} = 1 \\ (\sigma(H))}} | I_x g(H)_{\ell\ell} |$$

$$\leq \sup_{\|g\|_{L^\infty(\sigma(H))} = 1} \ \sup_{z \in \sigma(H)} | I_x g(z) |$$

$$= \sup_{z \in \sigma(H)} \sum_{x \in X_N} \underbrace{| \ell_x(z) |}_{\prod_{y \in X_N \setminus \{x\}} \frac{z-y}{x-y}}$$

Gauss Quadrature

$$D_\ell(x) \longrightarrow \begin{cases} p_n \in \mathcal{P}_n \quad \text{s.t.} \\ \int p_n(x)\, p_m(x)\, dD_\ell(x) = 0 \end{cases}$$

$$\downarrow$$

(Lanczos recursion)

T_N Cm

s.t. $X_N = \sigma(T_N)$

$$X_N := \{ x_0, \ldots, x_N \} = \text{roots of } p_{N+1}$$

$$\theta_\ell^N = \int I_{X_N} \circ \, dD_\ell = \int \circ \, dD_\ell^N$$

$$D_\ell^N = \sum_{x \in X_N} \ell_x(H)_{\ell\ell}\, \delta(\cdot - x)$$

Recursion method

$$O_\ell \approx o(T_N)_{00}$$

$$O_\ell^N = \Theta\left((H)_{\ell\ell}, \ldots, (H^{2N+1})_{\ell\ell} \right)$$

& $\Theta : U_N \subseteq \mathbb{C}^{2N+1} \to \mathbb{C}$ is analytic.

linear

$$|[o(H) - o^N(H)]_{\ell\ell}| \leq \| o - \boxed{o^N} \|_{\sigma(H)}$$

need knowledge of point spectrum

nonlinear

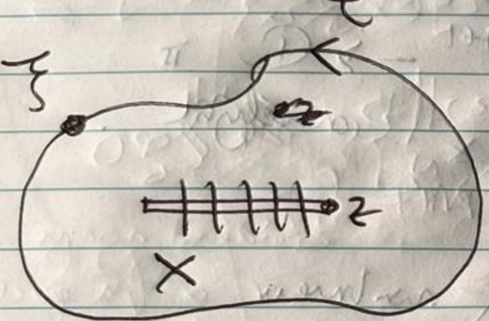
$$|O_\ell - O_\ell^N| \leq 2 \inf_{p \in \mathcal{P}_{2N+1}} \| o - p \|$$

$\ell^\infty(\sigma(H) \cup X_N)$

Why is the node polynomial important?

$$\ell_X = \prod_{x\in X} (z-x)$$

<u>Hermite</u> $z \in \mathbb{C}\setminus X$



$$O(z) - I_X O(z) = \oint_{\mathcal{C}} \frac{\ell_X(z)}{\ell_X(\xi)} \, \frac{O(\xi)}{\xi - z} \, d\xi$$

$$|O_\ell - O_\ell^N| \le C \sup_{\substack{z\in\sigma(H) \\ \xi\in\mathcal{C}}} \left| \frac{\ell_X(z)}{\ell_X(\xi)} \right|$$

choose X st

$$\boxed{\lim_{N\to\infty} \left| \frac{\ell_X(z)}{\ell_X(\xi)} \right|^{1/N} = e^{g(z)-g(\xi)}}$$

$$\left[\begin{array}{ll} \Delta g = 0 & \text{on } \mathbb{C}\setminus E \\ g \sim \log|z| & \text{as } |z|\to\infty \\ g = 0 & \text{on } E \end{array}\right]$$