Yserentant's results on the Regularity of Many-Electron Eigenfunctions

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All the science in this presentation was done by
***Harry Yserentant**, Mathematics, TU-Berlin*
and co-workers

H. Yserentant, Lecture Notes in Mathematics, **2000**, 2010
H. Yserentant, ESAIM: M2AN **45**, 803–824 (2011)
H.-C. Kreusler, H. Yserentant, Numer. Math., **121**, 781–802 (2012)

The electronic Schrödinger equation

Hamilton operator:

$$H \; = \; -\frac{1}{2}\sum_{i=1}^{N}\Delta_i - \sum_{i=1}^{N}\sum_{\nu=1}^{K}\frac{Z_\nu}{|\mathbf{x}_i - \mathbf{a}_\nu|} + \frac{1}{2}\sum_{\substack{i,j=1\\ i\neq j}}^{N}\frac{1}{|\mathbf{x}_i - \mathbf{x}_j|}$$

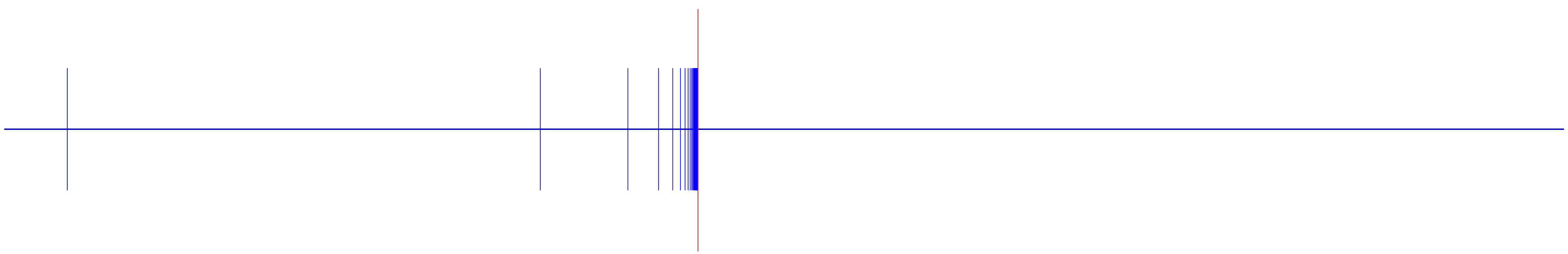
electronic eigenvalue problem:

$$Hu = \lambda u$$

The electronic Schrödinger equation

spectrum:

isolated eigenvalues $\lambda < \Sigma^*(\boldsymbol{\sigma}) \leq 0$, essential spectrum $\lambda \geq \Sigma^*(\boldsymbol{\sigma})$



here:

eigenfunctions for isolated eigenvalues $\lambda < \Sigma^*(\boldsymbol{\sigma})$

The electronic Schrödinger equation

solutions:

$$u \;:\; (\mathbb{R}^3)^N \to \mathbb{R} \;:\; (\mathbf{x}_1, \ldots, \mathbf{x}_N) \to u(\mathbf{x}_1, \ldots, \mathbf{x}_N)$$

depend on electron positions $\mathbf{x}_1, \ldots, \mathbf{x}_N \in \mathbb{R}^3$

water molecule:

H_2O : 3 nuclei, $N = 1{+}1{+}8$ electrons

u : $\mathbb{R}^{\mathbf{30}} \to \mathbb{R}$

The electronic Schrödinger equation

solutions (incl. spin):

$$u \;:\; (\mathbb{R}^3)^N \longrightarrow \mathbb{R} \;:\; (\mathbf{x}_1, \ldots, \mathbf{x}_N) \rightarrow \psi(\mathbf{x}_1, \ldots, \mathbf{x}_N; \boldsymbol{\sigma}_1, \ldots, \boldsymbol{\sigma}_N)$$

problem:

very high-dimensional domain, direct approximation possible?

rescue ?

Curse of dimensionality

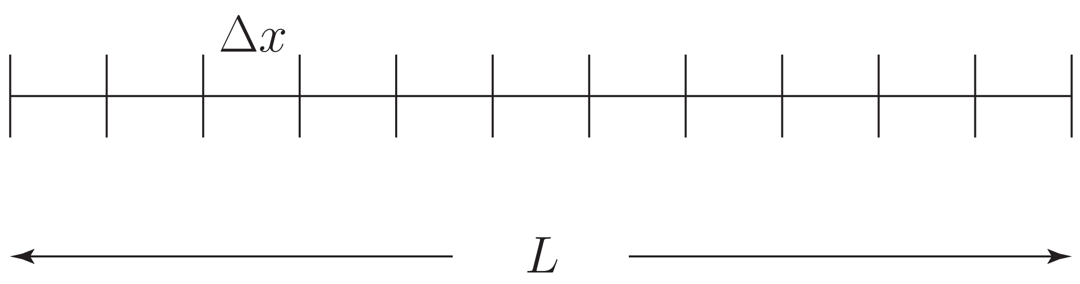
Error ε vs. number of degrees of freedom n in d dimensions

First order scheme

$$d = 1 \quad : \qquad \varepsilon \sim \frac{\Delta x}{L} \sim n^{-1}$$

$$d = 3 \quad : \qquad \varepsilon \sim \frac{\Delta x}{L} \sim n^{-1/3}$$

$$d = 3N : \qquad \varepsilon \sim \frac{\Delta x}{L} \sim n^{-1/3N}$$



Curse of dimensionality

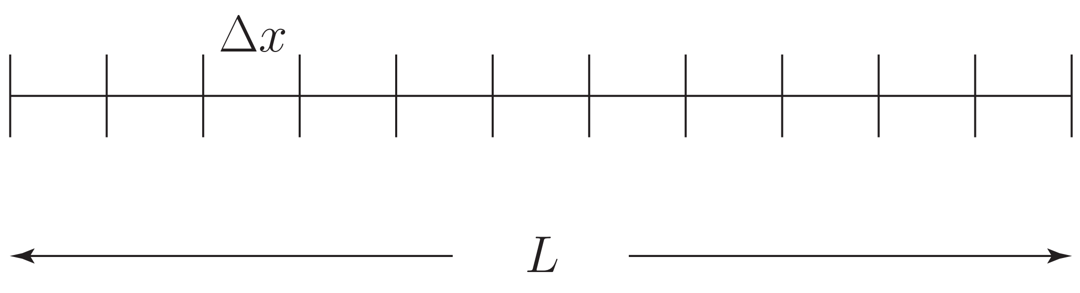
Error ε vs. number of degrees of freedom n in d dimensions

First order scheme $\varepsilon = \frac{1}{10}, \quad \Delta x/L = \frac{1}{10}, \quad N = 10$

$$d = 1 \quad : \quad \varepsilon \sim \frac{\Delta x}{L} \sim n^{-1} \qquad n \sim 10$$

$$d = 3 \quad : \quad \varepsilon \sim \frac{\Delta x}{L} \sim n^{\mathbf{-1/3}} \qquad n \sim 1\,000$$

$$d = 3N : \quad \varepsilon \sim \frac{\Delta x}{L} \sim n^{\mathbf{-1/3N}} \qquad n \sim 10^{30}$$



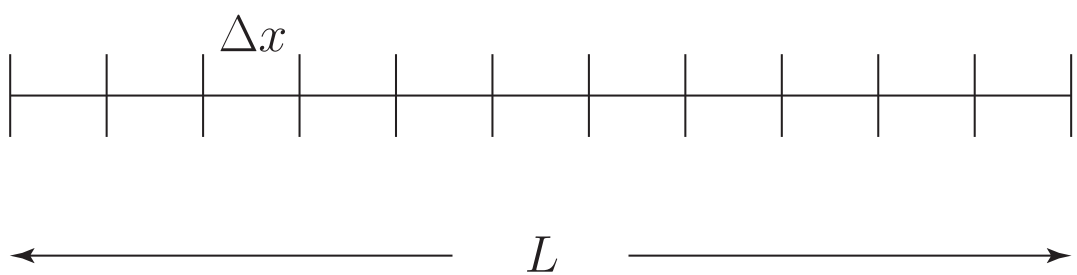
Curse of dimensionality

Error ε vs. number of degrees of freedom n in d dimensions

$\boldsymbol{p}$-th order scheme – requiring higher-order differentiability –

$$d = 1 \quad : \qquad \varepsilon \sim \left(\frac{\Delta x}{L}\right)^{\boldsymbol{p}} \sim n^{-\boldsymbol{p}}$$

$$d = 3N : \qquad \varepsilon \sim \left(\frac{\Delta x}{L}\right)^{\boldsymbol{p}} \sim n^{\underline{-\boldsymbol{p}/3N}} \qquad ?$$



Curse of dimensionality

What if Slater-determinants (or similar) did play a role ?

Suppose

$$u(\mathbf{x}) = \sum_{\mathbf{k}} \widehat{u}(\mathbf{k}) \left(\prod_{i=1}^{N} \phi_i(\mathbf{x}_i, \mathbf{k}_i) \right)^{*}$$

and the

$$\frac{\partial \phi_i}{\partial x_{i,\alpha}} \quad (\alpha \in \{1,2,3\}) \qquad \text{exist}$$

then the

N**-th order mixed derivatives** $\quad \frac{\partial}{\partial x_{1,\alpha_1}} \cdots \frac{\partial}{\partial x_{N,\alpha_N}} u \quad$ **should exist, too**

* anti-symmetrized & normalized

Curse of dimensionality

Why would this be note-worthy ?

Suppose we are in $d >> 1$ dimensions

$$u(\mathbf{x}) = \sum_{k_1>k_2\ldots>k_d} a(\mathbf{k})\phi(\mathbf{k},\mathbf{x}) \quad \text{with} \quad \phi(\mathbf{k},\mathbf{x}) = \left(\prod_{i=1}^{d} \sin(k_i x_i)\right)^{*}$$

and

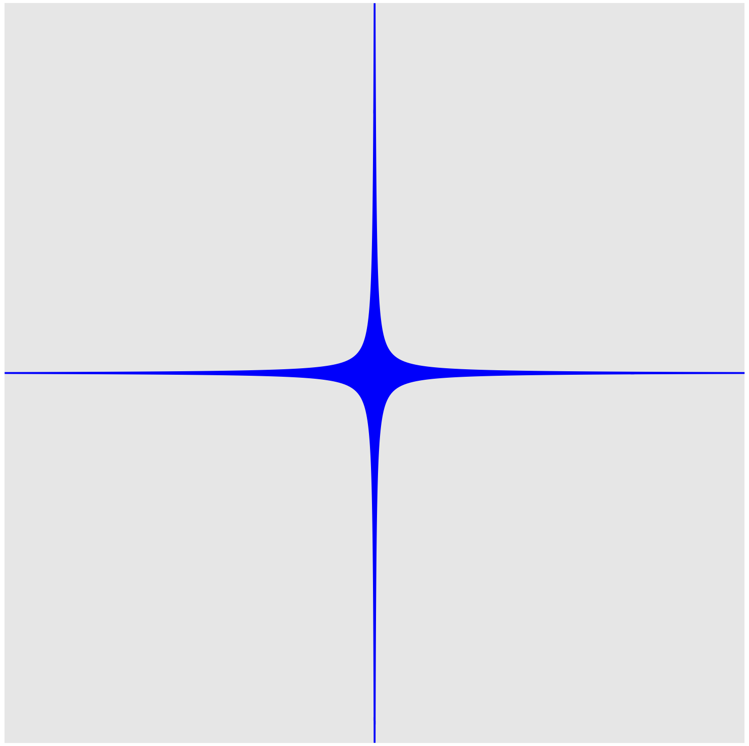
$$\left\| \frac{\partial}{\partial x_1} \ldots \frac{\partial}{\partial x_d} u \right\|_0^2 = \sum_{k_1>k_2\ldots>k_d} |\, k_1 \ldots k_d|^2 \, |\, a(\mathbf{k})|^2 < \infty$$

* anti-symmetrized & normalized

Curse of dimensionality

approximation space:

$$\mathcal{V}_L^a = \left\{ \sum_{k_1 > k_2 \ldots > k_d} a(\mathbf{k})\phi(\mathbf{k},\mathbf{x}) \;\middle|\; a(\mathbf{k}) = 0 \text{ for } |k_1 \ldots k_d| \geq 2^L \right\}$$



hyperbolic cross

Curse of dimensionality

approximation space:

$$\mathcal{V}_L^a = \Big\{ \sum_{k_1 > k_2 \ldots > k_d} a(\mathbf{k})\phi(\mathbf{k},\mathbf{x}) \;\Big|\; a(\mathbf{k}) = 0 \ \text{ for } \ |k_1 \ldots k_d| \geq 2^L \Big\}$$

dimension:

$$n = \dim \mathcal{V}_L^a \;\leq\; a(d,L) \;\leq\; (2^L)^{1+cL^{-1/2}}$$

approximation error:

$$\inf_{v \in \mathcal{V}_L^a} \|u - v\|_0 \;\leq\; \frac{1}{2^L} \Big\{ \sum_{\mathbf{k} \in \mathbb{N}^d} |k_1 \ldots k_d|^2 \, |\widehat{u}(\mathbf{k})|^2 \Big\}^{1/2}$$

$$= \frac{1}{2^L} \Big\| \frac{\partial}{\partial x_1} \cdots \frac{\partial}{\partial x_d} u \Big\|_0 \sim \underline{\left(\frac{1}{n}\right)^{1-O(L^{-1/2})}}$$

independent of d

The electronic Schrödinger equation

Hamilton operator:

$$H \;=\; -\frac{1}{2}\sum_{i=1}^{N}\Delta_i \;-\; \sum_{i=1}^{N}\sum_{\nu=1}^{K}\frac{Z_\nu}{|\mathbf{x}_i-\mathbf{a}_\nu|} + \frac{1}{2}\sum_{\substack{i,j=1\\ i\neq j}}^{N}\frac{1}{|\mathbf{x}_i-\mathbf{x}_j|}$$

eigenvalue problem:

$$Hu = \lambda u$$

The electronic Schrödinger equation

interaction potential:

$$V(\mathbf{x}) \;=\; -\sum_{i=1}^{N}\sum_{\nu=1}^{K}\frac{Z_\nu}{|\mathbf{x}_i-\mathbf{a}_\nu|} + \frac{1}{2}\sum_{\substack{i,j=1\\ i\neq j}}^{N}\frac{1}{|\mathbf{x}_i-\mathbf{x}_j|}$$

assigned bilinear form on H^1*:

$$a(u,v) \;=\; \int\Big\{\frac{1}{2}\nabla u\cdot\nabla v + Vuv\Big\}\,\mathrm{d}\mathbf{x}$$

weak formulation:

Find $u \in H^1$ with $a(u,v)=\lambda(u,v)$ for all $v\in H^1$

* H^1: functions v for which $\int v^2\,dx$ and $\int(\nabla v)^2\,dx$ are finite

Aside on variational formulation

For problems of this type

$$\text{Find} \quad u \in X \quad \text{with} \quad a(u,v) = \lambda(u,v) \quad \text{for all} \quad v \in X$$

or this, with $\boldsymbol{f} \in L_2$ *

$$\text{Find} \quad u \in X \quad \text{with} \quad a(u,v) = (\boldsymbol{f}, v) \quad \text{for all} \quad v \in X$$

coercivity plays the role of "invertibility" of matrices in finite dimensions

$$|a(u,v)| \le C_1 \|u\|_X \|v\|_X \qquad \text{boundedness, continuity}$$

$$|a(u,u)| \ge C_2 \|u\|_X^2 \qquad \text{akin to classical invertibility}$$

* square integrable

The electronic Schrödinger equation

interaction potential:

$$V(\mathbf{x}) \;=\; -\sum_{i=1}^{N}\sum_{\nu=1}^{K}\frac{Z_\nu}{|\mathbf{x}_i-\mathbf{a}_\nu|}+\frac{1}{2}\sum_{\substack{i,j=1\\ i\neq j}}^{N}\frac{1}{|\mathbf{x}_i-\mathbf{x}_j|}$$

three-dimensional Hardy inequality:

$$\int\frac{1}{|\mathbf{x}|^2}\,v^2\,\mathrm{d}\mathbf{x}\;\leq\;4\int|\nabla v|^2\,\mathrm{d}\mathbf{x}$$

estimate low-order part:

$$\int V u v\,\mathrm{d}\mathbf{x}\;\leq\;3\sqrt{N}\,\max(N,Z)\,\|u\|_0\|\nabla v\|_0$$

The electronic Schrödinger equation

Pauli principle:

Full, spin-dependent wave functions are antisymmetric with respect to the exchange of the electrons. Only solutions with certain symmetry properties are therefore admissible.

solution spaces $H^1(\boldsymbol{\sigma})$:

$$u \in H^1 \qquad \text{with} \qquad u(\mathbf{P}\mathbf{x}) = \operatorname{sign}(\mathbf{P})u(\mathbf{x}) \qquad \text{if} \qquad \mathbf{P}\boldsymbol{\sigma} = \boldsymbol{\sigma}$$

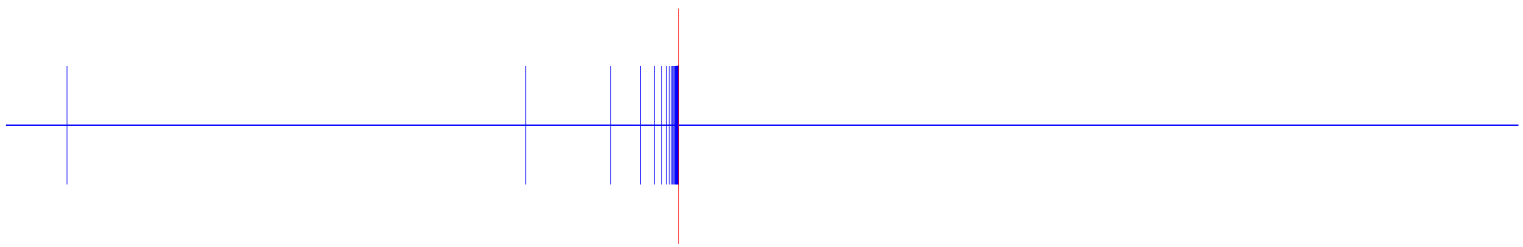
splitting of the full problem:

$$\text{Find} \qquad u \in H^1(\boldsymbol{\sigma}) \qquad \text{with} \qquad a(u,v) = \lambda(u,v) \qquad \text{for all} \qquad v \in H^1(\boldsymbol{\sigma})$$

Spectrum and exponential decay

spectrum:

isolated eigenvalues $\lambda < \Sigma^*(\boldsymbol{\sigma}) \leq 0$, essential spectrum $\lambda \geq \Sigma^*(\boldsymbol{\sigma})$

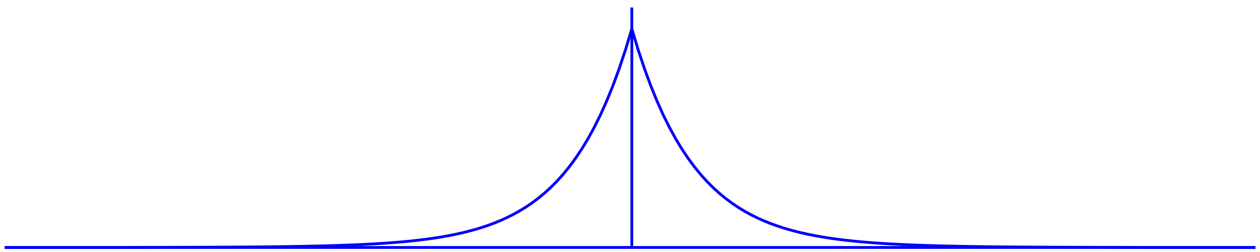


here:

eigenfunctions for isolated eigenvalues $\lambda < \Sigma^*(\boldsymbol{\sigma})$

Spectrum and exponential decay

hydrogen ground state $u(\mathbf{x}) = \mathrm{e}^{-Z|\mathbf{x}|}$, $\lambda = -\frac{1}{2}\,Z^2$:



multi-particle problem:

$$\exp\left(\gamma \sum_{i=1}^{N} |\mathbf{x}_i|\right) u(\mathbf{x}) \in H^1(\boldsymbol{\sigma}) \text{ for certain } \gamma > 0$$

Existence and decay of high derivatives

multi-indices:

$$\boldsymbol{\alpha} = (\boldsymbol{\alpha}_1, \ldots, \boldsymbol{\alpha}_N) \in (\mathbb{Z}^3_{\geq 0})^N, \quad \boldsymbol{\alpha}_i = (\alpha_{i,1}, \alpha_{i,2}, \alpha_{i,3}) \in \mathbb{Z}^3_{\geq 0}$$

(mixed) derivatives, monomials:

$$\mathrm{D}^{\boldsymbol{\alpha}} = \prod_{i=1}^{N} \prod_{\nu=1}^{3} \left(\frac{\partial}{\partial x_{i,\nu}} \right)^{\alpha_{i,\nu}}, \quad \mathbf{x}^{\boldsymbol{\alpha}} = \prod_{i=1}^{N} \prod_{\nu=1}^{3} x_{i,\nu}^{\alpha_{i,\nu}}$$

set of the here considered multi-indices:

$$\mathcal{A} \; = \; \left\{ (\boldsymbol{\alpha}_1, \ldots, \boldsymbol{\alpha}_N) \,\middle|\, \boldsymbol{\alpha}_i \in \mathbb{Z}^3_{\geq 0},\ \alpha_{i,1} + \alpha_{i,2} + \alpha_{i,3} \leq 1 \right\}$$

Existence and decay of high derivatives

regular parts of the eigenfunctions:

$$u_0(\mathbf{x}) \;=\; \exp\left(2\sum_{i,\nu} Z_\nu\,\phi(\mathbf{x}_i-\mathbf{a}_\nu)\;-\sum_{i<j}\phi(\mathbf{x}_i-\mathbf{x}_j)\right)u(\mathbf{x})$$

example for the choice of ϕ:

$$\phi(\mathbf{x}) \;=\; \ln\left(1+\frac{1}{2}\,|\mathbf{x}|\right)$$

Existence and decay of high derivatives

regular parts:

$$u_0(\mathbf{x}) \,=\, \exp\left(2\sum_{i,\nu} Z_\nu\,\phi(\mathbf{x}_i - \mathbf{a}_\nu) \,-\, \sum_{i<j}\phi(\mathbf{x}_i - \mathbf{x}_j)\right) u(\mathbf{x})$$

central result:

The regular parts u_0 of the eigenfunctions u possess weak derivatives $\mathrm{D}^{\boldsymbol{\alpha}} u_0$ for all multi-indices $\boldsymbol{\alpha} \in \mathcal{A}$. Moreover,

$$\exp\left(\gamma\sum_{i=1}^{N}|\mathbf{x}_i|\right)(\mathrm{D}^{\boldsymbol{\alpha}} u_0)(\mathbf{x}) \,\in\, H^1$$

with the same $\gamma > 0$ as for the eigenfunctions themselves.

Idea of proof

exponentially weighted regular parts:

$$\widetilde{u}(\mathbf{x}) \;=\; \exp\left(\gamma \sum_{i=1}^{N} |\mathbf{x}_i|\right) u_0(\mathbf{x})$$

second-order equation:

$$\frac{1}{2}\int \nabla\widetilde{u}\cdot\nabla v \,\mathrm{d}\mathbf{x} \;+\; s(\widetilde{u}, v) \;=\; \lambda\,(\widetilde{u}, v), \quad v \in H^1$$

estimate for low-order part:

$$s(u, v) \;\lesssim\; \|u\|_1 \|v\|_0, \quad u, v \in H^1$$

Idea of proof

frequency decomposition $\widetilde{u} = u_L + u_H$:*

$$\frac{1}{2}\int \nabla u_H \cdot \nabla \chi_H \, \mathrm{d}\mathbf{x} + s(u_H, \chi_H) - \lambda\,(u_H, \chi_H) = -\, s(u_L, \chi_H), \quad \chi_H \in H^1_H$$

high-frequency parts:

$$\|u_H\|_0 \le \Omega^{-1} \|\nabla u_H\|_0$$

estimate for low-order part:

$$s(u,v) \lesssim \|u\|_1 \|v\|_0, \quad u, v \in H^1$$

* u_L: $\widehat{u}(\mathbf{k})$ for $|\mathbf{k}| \le \Omega$, u_H: $\widehat{u}(\mathbf{k})$ for $|\mathbf{k}| > \Omega$

Idea of proof

equation of order $2N+2$:

$$\frac{1}{2}\int \nabla\widetilde{u}\cdot\nabla\mathcal{L}v\,\mathrm{d}\mathbf{x} + s(\widetilde{u},\mathcal{L}v) = \lambda\,(\widetilde{u},\mathcal{L}v), \quad v\in\mathcal{S}$$

$$\mathcal{L} := \prod_{i=1}^{N}(I-\Delta_i)$$

key property:

$$s(u,\mathcal{L}v) \lesssim \sum_{\boldsymbol{\alpha}\in\mathcal{A}} \|\mathrm{D}^{\boldsymbol{\alpha}}u\|_0\|\mathrm{D}^{\boldsymbol{\alpha}}v\|_1, \quad u,v\in\mathcal{S}$$

$\mathcal{S}$ = rapidly decreasing functions

Approximation of the eigenfunctions

representation of the eigenfunctions:

$$u(\mathbf{x}) \;=\; \exp\left(-\,2\sum_{i,\nu} Z_\nu\,\phi(\mathbf{x}_i-\mathbf{a}_\nu)\;+\;\sum_{i<j}\phi(\mathbf{x}_i-\mathbf{x}_j)\right)u_0(\mathbf{x})$$

$$\exp\left(\gamma\sum_{i=1}^{N}|\mathbf{x}_i|\right)(\mathrm{D}^{\boldsymbol{\alpha}}u_0)(\mathbf{x}) \;\in\; H^1 \quad \text{for all } \boldsymbol{\alpha}\in\mathcal{A}$$

Approximation of the eigenfunctions

representation of the eigenfunctions:

$$u(\mathbf{x}) \;=\; \exp\left(-\,2 \sum_{i,\nu} Z_\nu\, \phi(\mathbf{x}_i - \mathbf{a}_\nu) \,+\, \sum_{i<j} \phi(\mathbf{x}_i - \mathbf{x}_j) \right) u_0(\mathbf{x})$$

approximate eigenfunctions:

$$u(\mathbf{x}) \;\approx\; \exp\left(-\,2 \sum_{i,\nu} Z_\nu\, \phi(\mathbf{x}_i - \mathbf{a}_\nu) \,+\, \sum_{i<j} \phi(\mathbf{x}_i - \mathbf{x}_j) \right) v(\mathbf{x})$$

ansatz for the regular part v:

antisymmetrized sparse grid functions
based on three-dimensional function systems*

* Eigenfunctions of one-particle Hamiltonians!!

DE
PARTITIONE NVMERORVM.
AVCTORE
L. EVLERO.

§. 1.

Problema *de partitione numerorum* primum mihi eſt propoſitum a *Celeb. Profeſſore Haude*, in quo quaerebat, quot variis modis datus numerus integer, (hic enim perpetuo de numeris tantum integris et affirmatiuis eſt ſermo,) poſſit eſſe aggregatum, duorum vel trium vel quatuor, vel in genere quot libuerit numerorum. Siue quod eodem redit, quaeritur, quot variis modis datus numerus vel in duas, vel tres, vel quatuor, vel quot libuerit partes

ASYMPTOTIC FORMULÆ IN COMBINATORY ANALYSIS

By G. H. HARDY AND S. RAMANUJAN.*

[Preliminary communication December 14th, 1916.—Read January 18th, 1917.—
Received February 28th, 1917.]

1.

INTRODUCTION AND SUMMARY OF RESULTS.

1.1. The present paper is the outcome of an attempt to apply to the principal problems of the theory of partitions the methods, depending upon the theory of analytic functions, which have proved so fruitful in the theory of the distribution of primes and allied branches of the analytic theory of numbers.

The most interesting functions of the theory of partitions appear as the coefficients in the power-series which represent certain elliptic modular functions. Thus $p(n)$, the number of unrestricted partitions of n, is the

Complexity of the N-electron problem

sparse grid approximation:

To obtain an H^1-error of order $\mathcal{O}(1/n)$, one needs asymptotically at most $\mathcal{O}(n^{3+\vartheta})$ correspondingly antisymmetrized sparse grid functions, where $\vartheta > 0$ can be chosen arbitrarily small.

That is, independent of N, the error of the best n-term approximation tends to zero almost like

$$\varepsilon \sim n^{\mathbf{-1/3}}$$

... which was the complexity of the single-particle problem!

The electronic Schrödinger equation

solutions (incl. spin):

$$u \; : \; (\mathbb{R}^3)^N \rightarrow \mathbb{R} \; : \; (\mathbf{x}_1, \ldots, \mathbf{x}_N) \rightarrow \psi(\mathbf{x}_1, \ldots, \mathbf{x}_N; \boldsymbol{\sigma}_1, \ldots, \boldsymbol{\sigma}_N)$$

problem:

very high-dimensional domain, direct approximation possible?

rescue:

N-th order mixed derivatives exist and decay exponentially

smoothness increases with number of electrons

symmetry properties enforced by the Pauli principle

Yserentant's results on the Regularity of Many-Electron Eigenfunctions

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