Computing Energy Levels of the Confined Hydrogen Atom

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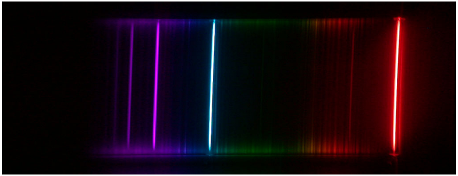
Thesis Proposal

- studying the physical system
  - statistical mechanics
  - time invariant Schrödinger equation (TISE)
  - confined hydrogen atom
- studying eigenvalue methods for large sparse systems
  - Lanczos and Jacobi-Davidson methods
- discretising the TISE
- implementing an eigenvalue algorithm
- computing the eigenvalues of the confined hydrogen atom

The Hydrogen Atom

- most simple atom
- single proton and single electron
- model for more complex atoms
- application in
  - chemistry
  - solid state physics
  - plasma physics
- Energy Levels
  - correspond to emission lines
  - set of discrete wave length
  - set of emission lines is called spectrum



The Time Invariant Schrödinger Equation

- energy levels correspond to eigenvalues of the TISE
- formulated by Schrödigner in 1926

$$\frac{1}{2}\Delta\psi(x) + \frac{1}{||x||}\psi(x) = \lambda\psi(x) \tag{1}$$

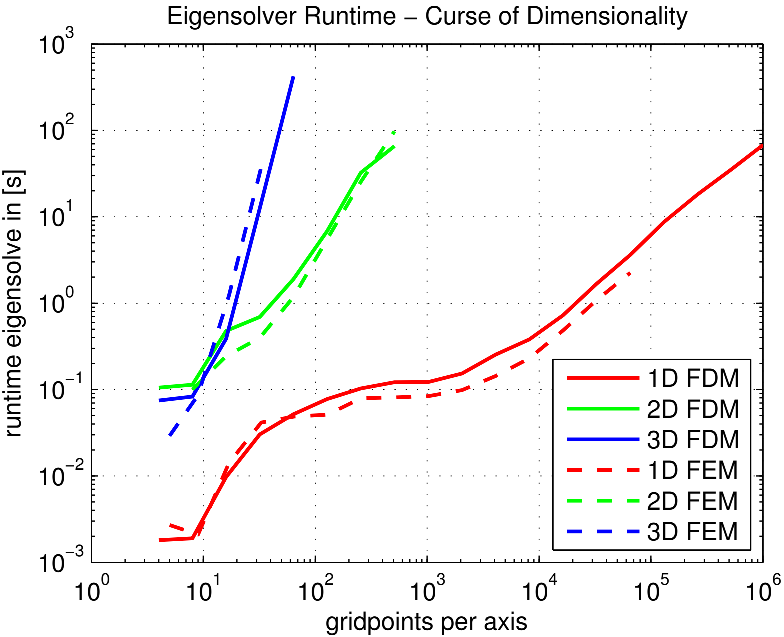
- time invariant
- non-relativistic
- singular potential
- elliptic boundary value problem with Dirichlet boundary conditions

Why are we here?

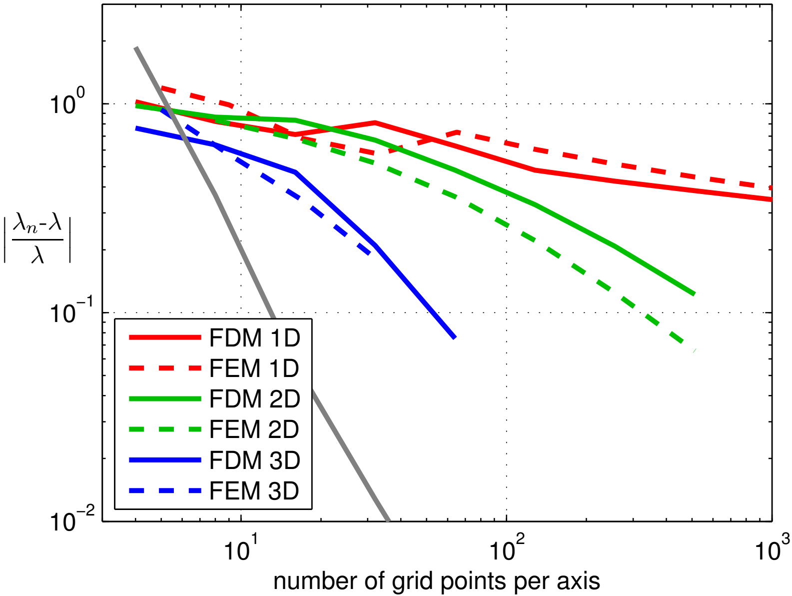
Find numerical answers to physical questions

- accurate
- efficient

Efficiency - Run time of the Arpack Eigensolver



Accuracy - Discretisations Error with Uniform Grids



What can be improved?

Run time

$$t \approx c_t n^d \qquad (2)$$

Discretisation Error

$$e \approx c_e \frac{1}{n^p} \qquad (3)$$

Smarter Discretisation (h, r and p-adaptivity)

- variable grid and adaptive meshes
- sparse grid
- Richardson extrapolation
- higher order discretisation
- spectral methods

Smarter Solvers

- faster algorithm
- faster implementation of exisisting algorithms (SIMD,SMP,GPU)

Improving Accuracy - Variable Grids and Adapted Meshed

Discretisation error estimates

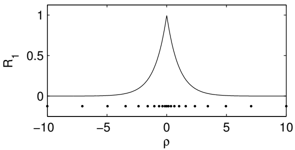
$$e_{FDM} = C_{FDM} h^2 \Psi^{(vi)} + O(h^4) \qquad ||e_{FEM}|| \leq C_{FEM} h^2 ||\Psi''|| \quad (4)$$

- Eigenfunctions of the hydrogen atom decay exponetially
- So do the derivatives
- Refine mesh close to nucleus to improve accuracy

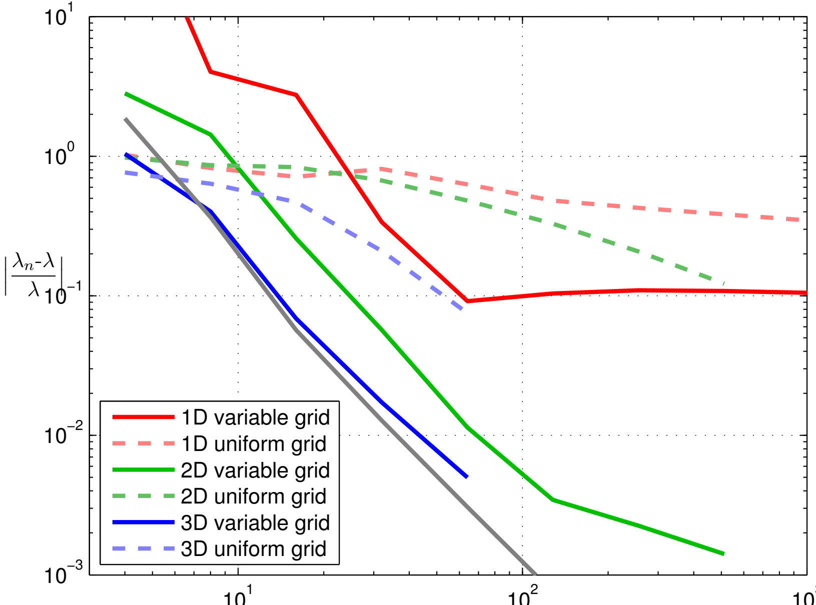
$$R_1 = \frac{1}{\sqrt{\pi}} exp(-\rho) \qquad (5)$$

$$R_1 = R_1'' = R_1^{(iv)} \qquad (6)$$

$$\tilde{x}_i \leftarrow \alpha_1 (exp(\alpha_2 x) - 1) \qquad (7)$$



Improving Accuracy - Discretisation Error with Variable Grids



Energy Levels of the Unconfined Atom

Formula

$$E = \frac{-2}{(2(n+1)+d-3)^2} \tag{8}$$

Energy Levels (E) and Degeneracy (g)

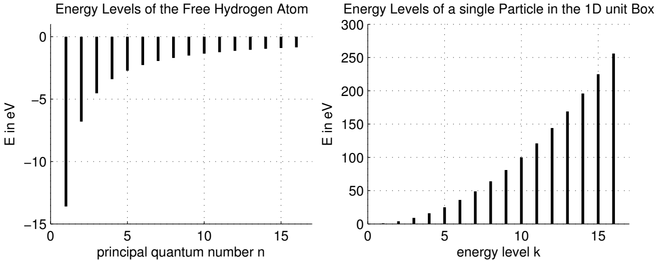
3D		2D		1D	
E	g	E	g	E	g
-0.5000	1	-2.0000	1	-Inf	1
-0.1250	4	-0.2222	3	-0.5000	2
-0.0556	9	-0.0800	5	-0.1250	2
-0.0312	16	-0.0408	7	-0.0556	2
-0.0200	25	-0.0247	9	-0.0312	2

The Confined Hydrogen Atom

Extension of hydrogen wave functions

State	$r_{P_{max}}$	$r_{10^{-15}}$
100	1.00	34
200	5.23	73
300	13.07	125

- wafe functions of higher energy levels reach further
- confinement influences higher energy levels more severely
- negative bound states become positive unbound states



Energy Levels of the Confined Two Dimensional Hydrogen Atom

Number of negative bound states (m)

L_0	1	2	4	8	16	32	∞
m	0	1	1	4	6	16	∞

Partition Function

$$Z = \sum exp(-\beta\lambda) \tag{9}$$

Value of the partition function at T=1000K

L_0	1	1.1	1.2	1.3	1.4	1.5	1.6	1.7	1.8	1.9	2.0
$log_{10}Z$	-Inf	-539	-278	-85	60	171	258	325	379	421	455

Z shows sudden transition from divergence to convergence

Thesis Prospect

- Improving accuracy of the dicretisation
  - adaptive FDM / FEM
  - investigation of convergence in case of confinement
- Eigenvalue Solvers
  - choosing an appropriate solver
  - testing existing implementations
  - implementing a solver on a GPU/SMP system
- Answering Physical research questions
  - size of cavity
  - location of nucleus
  - aspect ratio of the cavity
  - elliptic vs rectangular cavities
  - limit cases towards 2D and 1D
  - relation to unconfined and spherically confined H-atom
  - influence on the partition function