Imaginary time propagation code for large-scale two-dimensional eigenvalue problems in magnetic fields

P. J. J. Luukko[1,*], E. Räsänen[2]

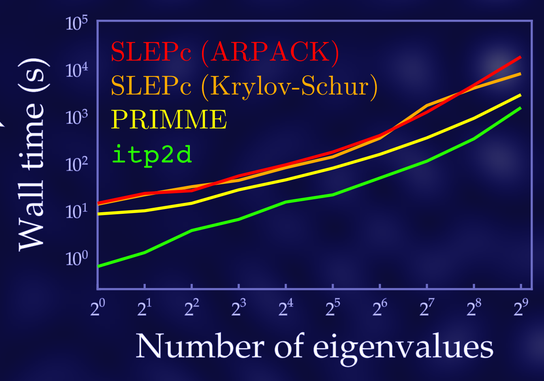
[1] Nanoscience Center, University of Jyväskylä, FI-40014, Jyväskylä, Finland
[2] Department of Physics, Tampere University of Technology, FI-33101 Tampere, Finland
[*] perttu.luukko@iki.fi

Introduction

We present `itp2d` – our code [1,2] for solving the single-particle, time-independent Schrödinger equation in 2D.

The code is based on the imaginary time propagation (ITP) method (aka split operator method), with its most recent developments:
— Arbitrary high order operator factorization [3]
— Exact inclusion of a (possibly strong) external magnetic field [4]

Our emphasis:
— Modern, easily extensible design
— Open-source development
— Not compromising speed!



Our aim:
— Single, versatile code for all Schrödinger-solving needs
— Statistical properties of energy levels, Quantum chaos
— Real-space code for disordered, noisy systems with no symmetry

Our implementation

— Implemented in C++ with a modern, object-oriented design
— Open source, freely available [2]
— Documentation & Python scripts for data analysis included

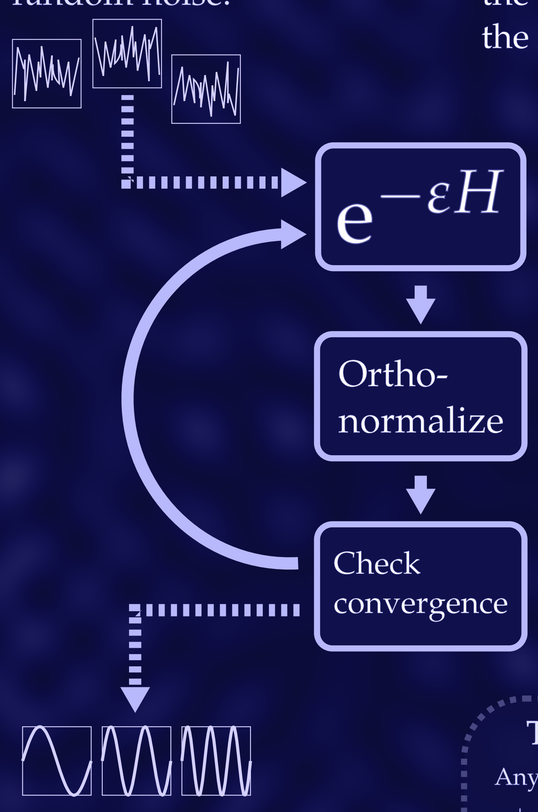
— Real space rectangular grid
— Periodic or Dirichlet boundary conditions
— Easy to implement arbitrary local potentials
— To model realistic systems, random impurities can be added
— Tech keywords: CBLAS, LAPACK, OpenMP, FFTW, HDF5

— The imaginary time propagation operator $e^{-\varepsilon H}$ is factorized to parts involving pointwise products, sums and discrete Fourier transforms. This factorization can be done to any order in ε [3]
— The Hamiltonian can include a homogeneous magnetic field perpendicular to the plane, and this field can be strong [4]
— Orthonormalization is done with a fast in-place implementation of the Löwdin algorithm

The ITP method

Input: An initial guess for the states. Can be simply random noise.

In iterations of ITP higher energy components are "shaved off" from the states step by step. In the end only the N lowest energy eigenstates remain.



Step 1: Propagate each state with the imaginary time propagation operator. The resulting states have less higher energy components.

Step 2: Orthonormalize the states. This preserves the N lowest energy components.

Step 3: Check for convergence by e.g. computing the variance with respect to the Hamiltonian H.

Output: The set of N lowest energy eigenstates of H.

The essential math:

Any arbitrary state can be expanded in the eigenstates of H

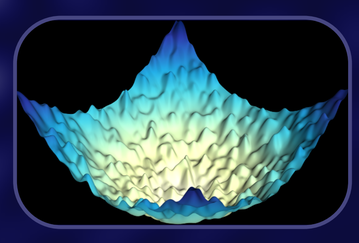
$$|\phi\rangle = \sum_i c_i |\psi_i\rangle$$

The ITP operator diminishes each component depending on the energy.

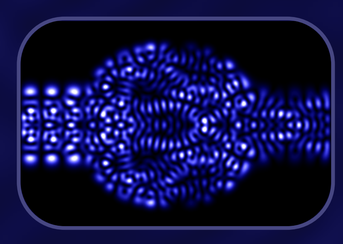
$$e^{-\varepsilon H}|\phi\rangle = \sum_i c_i e^{-\varepsilon H}|\psi_i\rangle = \sum_i c_i e^{-\varepsilon E_i}|\psi_i\rangle$$

Future prospects

Energy level statistics of disordered and noisy quantum dots and billiard systems: ideal for our real-space code.



Using the large eigenbasis provided by `itp2d` for transport calculations with the Landauer formalism
— Transport through systems with impurities, complicated potentials, strong magnetic fields...



Coupling with the Kohn–Sham scheme in density-functional theory for many-particle calculations.

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References

[1] P. J. J. Luukko, E. Räsänen, Comput. Phys. Commun. **184**, 769 (2013)
[2] `https://bitbucket.org/luukko/itp2d`
[3] S. A. Chin, Celest. Mech. Dyn. Astron. **106**, 391 (2010)
[4] M. Aichinger *et al*, Comput. Phys. Commun. **171**, 197 (2005)

Showcase: particle in a box with a strong magnetic field, eigenstate densities, highly excited states