



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

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ABSTRACT

We present a code for solving the single-particle, time-independent Schrödinger equation in two dimensions. Our program utilizes the imaginary time propagation (ITP) algorithm, and it includes the most recent developments in the ITP method: the arbitrary order operator factorization and the exact inclusion of a (possibly very strong) magnetic field. Our program is able to solve thousands of eigenstates of a two-dimensional quantum system in reasonable time with commonly available hardware. The main motivation behind our work is to allow the study of highly excited states and energy spectra of two-dimensional quantum dots and billiard systems with a single versatile code, e.g., in quantum chaos research. In our implementation we emphasize a modern and easily extensible design, simple and user-friendly interfaces, and an open-source development philosophy.

Program summary

Program title: itp2d

Catalogue identifier: AENR_v1_0

Program summary URL: http://cpc.cs.qub.ac.uk/summaries/AENR_v1_0.html

Program obtainable from: CPC Program Library, Queen's University, Belfast, N. Ireland

Licensing provisions: GNU General Public License version 3

No. of lines in distributed program, including test data, etc.: 11310

No. of bytes in distributed program, including test data, etc.: 97720

Distribution format: tar.gz

Programming language: C++ and Python.

Computer: Tested on x86 and x86-64 architectures.

Operating system: Tested under Linux with the g++ compiler. Any POSIX-compliant OS with a C++ compiler and the required external routines should suffice.

Has the code been vectorised or parallelized?: Yes, with OpenMP.

RAM: 1 MB or more, depending on system size.

Classification: 7.3.

External routines: FFTW3 (<http://www.fftw.org>), CBLAS (<http://netlib.org/blas>),

LAPACK (<http://www.netlib.org/lapack>), HDF5 (<http://www.hdfgroup.org/HDF5>),

OpenMP (<http://openmp.org>), TCLAP (<http://tclap.sourceforge.net>), Python (<http://python.org>),

Google Test (<http://code.google.com/p/googletest/>)

Nature of problem: Numerical calculation of the lowest energy solutions (up to a few thousand, depending on available memory), of a single-particle, time-independent Schrödinger equation in two dimensions with or without a homogeneous magnetic field.

Solution method: Imaginary time propagation (also known as the diffusion algorithm), with arbitrary even order factorization of the imaginary time evolution operator

Additional comments: Please see the README file distributed with the program for more information. The source code of our program is also available at <https://bitbucket.org/luukko/itp2d>.

Running time: Seconds to hours

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[☆] This paper and its associated computer program are available via the Computer Physics Communication homepage on ScienceDirect (<http://www.sciencedirect.com/science/journal/00104655>).

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1. Introduction

In this paper we present itp2d: a modern implementation of the imaginary time propagation (ITP) scheme for solving the eigenstates of a two-dimensional, single-particle quantum system

from the time-independent Schrödinger equation. Our implementation includes the most recent developments in imaginary time propagation, namely, the arbitrary order operator factorization by Chin [1], and the exact method of including a homogeneous magnetic field developed by Aichinger et al. [2,3].

The computational methods used in our program have been implemented before [4,2,5], but `itp2d` is the first to combine them all in a two-dimensional code. In addition, with `itp2d` we focus on a clear, object-oriented, and extensible implementation, without compromising efficiency. We have also emphasized on making the implementation suitable for solving a great number of eigenstates – up to thousands – in reasonable time. With this we intend to make `itp2d` a useful tool for studying the energy level spectra and highly excited wave functions of two-dimensional quantum systems, for example in the field of quantum chaos [6]. Since solving the single-particle equation is also a crucial part in the many-particle formalism of density-functional theory, `itp2d` can also be used as a fast eigensolver for realistic electronic structure calculations.

There are other algorithms designed for probing the highly excited states of quantum billiards, such as the various boundary methods (see, e.g. Refs. [7,8] and references therein), but we have chosen ITP for its versatility and its ability to handle strong magnetic fields. To our knowledge, ITP with its latest developments has not been thoroughly benchmarked against other general-purpose iterative eigensolvers. In one reported case [9], ITP was found to have a much better scalability with respect to the grid size compared to the Lanczos method, but worse scalability with respect to the number of states. However, these conclusions were based on a single 3D system solved only up to 10 eigenstates with the older, 4th order operator factorization. In Section 4.3 we present benchmark results which indicate that `itp2d` provides competitive numerical efficiency compared to publicly available, general-purpose eigensolvers.

ITP can and has been [4] implemented in any number of dimensions. We have chosen to limit our implementation to two dimensions for simplicity, and because operating in two dimensions allows systems with thousands of eigenstates to fit into system RAM, minimizing slow I/O operations.

In order to give a reasonably self-contained presentation, we will first introduce the ITP scheme and the underlying algorithms used in our implementation. A reader who is already familiar with ITP can advance directly to Section 3, where we will describe the implementation in more detail.

All formulas in this paper are given in Hartree atomic units. The magnetism-related units follow the SI-based convention, i.e., the atomic unit of magnetic field is \hbar/ea_0^2 , where e is the unit charge and a_0 is the Bohr radius.

2. Algorithms

2.1. Imaginary time propagation

Imaginary time propagation (also known as the *diffusion method*) is a general algorithm for solving eigenvalue problems such as the time-independent Schrödinger equation

$$H\psi = E\psi,$$

where H is the Hamiltonian of the system, and the solution of the eigenvalue problem is some set of energies $\{E_j\}$ and the associated eigenstates $\{\psi_j\}$.

The ITP algorithm is based on the idea that the (initially unknown) eigenstates of H form a complete basis of the associated Hilbert space, and thus any arbitrary state ϕ can be expanded in the eigenstates of H as

$$\phi = \sum_j c_j \psi_j,$$

where $\{c_j\}$ is some set of coefficients. By choosing an operator $\mathcal{T} = \exp(-\varepsilon H)$, where $\varepsilon > 0$, we can “filter out” the lower energy states out of this expansion by repeatedly applying \mathcal{T} to our initial state ϕ . After one iteration we get

$$\mathcal{T}\phi = \sum_j c_j \mathcal{T}\psi_j = \sum_j (c_j \exp(-\varepsilon E_j)) \psi_j, \quad (1)$$

in other words, components in the expansion are damped with the damping coefficient approaching zero exponentially with increasing energy and increasing value for ε . By repeatedly applying the operator \mathcal{T} and subsequently normalizing the state, all higher energy components are removed from the expansion and only the ground state of the Hamiltonian remains. The operator \mathcal{T} has the same form as the time evolution operator of a quantum system in the Schrödinger picture, $\exp(-itH)$, only with an imaginary number inserted for time, giving the ITP algorithm its name. For this reason the value ε is also called the *imaginary time step*.

In order to get more states besides the ground state one chooses a set of arbitrary, linearly independent initial states and repeatedly applies \mathcal{T} on each state followed by orthonormalizing the set of states. By choosing a set of N initial states this procedure leads to the set of N lowest energy eigenstates of the Hamiltonian. The convergence speed of each state typically depends on its energy, with the ground state converging first and the highest energy states last. This also means that often it is advantageous to include some extra states in the computation – with more states each iteration takes longer, but since the absolutely highest states are not required to converge, the number of required iterations is reduced.

Since the method is based on removing unwanted components to project out the wanted ones, it is essential that the initial states really include all desired components in the first place, i.e., even though the initial states are otherwise arbitrary, all of them should not be orthogonal to any eigenstate. A simple way to make sure that this requirement is practically always fulfilled is to choose random noise as the initial states.

To apply the ITP method in computer simulations we need a method to compute $\mathcal{T}\phi$ for an arbitrary state ϕ , an efficient method to orthonormalize a set of states, and a method to check for convergence, i.e. to assess whether the current set of states is close enough to the true eigenstates of H . After these steps are implemented the iterative ITP scheme can be used as summarized in the following:

1. Start with a set of N arbitrary, linearly independent states ϕ_n .
2. Apply the operator $\mathcal{T} = \exp(-\varepsilon H)$ to each state.
3. Orthonormalize the set of states.
4. Check whether convergence has been achieved. If yes, terminate, if not, go back to step 2.

2.2. Orthonormalization

The orthonormalization of states can be executed with a standard Gram–Schmidt process, but in our implementation we have opted for the Löwdin orthonormalization algorithm [10] (also known as subspace orthonormalization), which has been shown to be better suited for ITP in previous implementations [5]. In the Gram–Schmidt method one state is chosen to be a starting point of the iterative orthonormalization scheme, whereas the Löwdin method treats all states equally. Furthermore, it has been shown [11] that among a very general family of orthonormalization procedures, the Löwdin algorithm is the algorithm that changes the states the *least* in terms of the root-mean-square distance between the initial and orthonormalized states. This “minimal disturbance” property of the Löwdin algorithm is useful for smooth convergence in the ITP scheme.

The Löwdin method for orthonormalizing a set $\{\phi_j\}$ of N linearly independent states can be summarized as follows. First the overlap matrix M with $M_{ij} = \langle \phi_i | \phi_j \rangle$ is computed. Then the Hermitian matrix M is diagonalized, which results in a unitary matrix U and a diagonal matrix $D = \text{diag}(m_1, m_2, \dots, m_N)$ such that $M = UDU^\dagger$. Now the linear combinations

$$\phi'_i = \frac{1}{\sqrt{m_i}} \sum_j U_{ji} \phi_j \quad (2)$$

form an orthonormalized set, which can be confirmed easily by a direct calculation of the inner product $\langle \phi'_i | \phi'_j \rangle$. In total, the Löwdin algorithm for N states amounts computationally to

1. Computing $N(N + 1)/2$ inner products to form the overlap matrix M
2. Diagonalizing a $N \times N$ Hermitian matrix M
3. Forming the linear combinations (2) which, if the states are stored as N arrays of M numbers each, amounts to the computation of a matrix product between a $N \times N$ unitary matrix and a $N \times M$ matrix.

All these steps can be implemented easily and efficiently with standard linear algebra routines. In addition, all these steps can be computed without allocating memory for a second set of states.

The Löwdin orthonormalization also provides a way to approximate the energy of each state based on the eigenvalues $\{m_n\}$, since with successive iterations $m_n \rightarrow \exp(-2\varepsilon E_n)$. However, in systems with a high number of states, the energy values E_n become very large, which causes the values for m_n get very close to zero. In turn, the accuracy of this approximation becomes quite poor.

Regardless of the algorithm used, a requirement for orthonormalization to work is of course that the states are linearly independent. This can be asserted for the initial states, but it can happen that the states lose linear independence during the propagation. If the states are propagated with a too large time step several states can, for example, get so close to the ground state that they are essentially linearly dependent. This poses limitations on how large time steps can be used.

2.3. Factorization of the imaginary time evolution operator

For practical Hamiltonians the exponential $\mathcal{T} = \exp(-\varepsilon H)$ can not be implemented directly in computations. The traditional approach to this problem is to approximately factorize the exponential into an easier form. For a Hamiltonian of the form $H = T + V$, the most simple approximation is the second-order factorization

$$\mathcal{T} = \exp\left(-\frac{1}{2}\varepsilon V\right) \exp(-\varepsilon T) \exp\left(-\frac{1}{2}\varepsilon V\right) + \mathcal{O}(\varepsilon^3). \quad (3)$$

If T represents the kinetic energy operator, $T \propto \nabla^2$, and V is a local potential operator, both remaining exponentials $\exp(-\frac{1}{2}\varepsilon V)$ and $\exp(-\varepsilon T)$ can be implemented easily: the exponential of V is still a local potential, so in the coordinate basis it is diagonal, and likewise the exponential of T is diagonal in the wave vector basis. This means that for wave functions in the coordinate basis an exponential of V is simply a pointwise multiplication, and an exponential of T is a combination of a Fourier transform and a pointwise multiplication.

As pointed out, the factorization in Eq. (3) is only approximate for general Hamiltonians. When using an approximate evolution operator \mathcal{T}' , we essentially replace the original Hamiltonian H with an approximation H' such that $\mathcal{T}' = \exp(-\varepsilon H')$, and the eigenstates we get with the ITP method are actually the eigenstates of H' . The better the approximation for \mathcal{T} , the more accurately the eigenenergies and eigenstates of H' match the true result we would

get for H . Since some kind of approximation for \mathcal{T} is required we need to find a balance between two opposing effects when choosing a value for the imaginary time step ε : a larger value for ε causes the ITP scheme to converge *faster* (as seen directly from the “damping factor” in Eq. (1)), but the ε -dependent approximation causes the scheme to converge *further away* from the true solution.

In order to improve the ITP method, several improved, higher order approximations for \mathcal{T} have developed beyond the second-order factorization of Eq. (3). The most recent improvement is the factorization by Chin [1], that constructs an *arbitrarily high order* approximation for \mathcal{T} from the second-order factorization:

$$\mathcal{T} = \sum_{k=1}^n c_k \mathcal{T}_2^k(\varepsilon/k) + \mathcal{O}(\varepsilon^{2n+1}), \quad (4)$$

where $\mathcal{T}_2(\varepsilon)$ is the second-order approximation from Eq. (3), and the coefficients $\{c_i\}$ are given by

$$c_i = \prod_{\substack{j=1 \\ j \neq i}}^n \frac{i^2}{i^2 - j^2}.$$

Using a higher-order approximation for \mathcal{T} allows for higher values of ε , which improves the convergence rate of the ITP scheme. This is highly advantageous, since even though more complicated approximations for \mathcal{T} make the propagation step more computationally intensive, fewer iterations are needed due to the faster convergence rate. As the number of states N is increased, the computational cost of the propagation step in the ITP scheme scales as $\propto N$ (each state is simply propagated independently of the others), but the orthonormalization step usually scales as $\propto N^2$ or worse. This means that regardless of how complicated the propagation operator \mathcal{T} is, the orthonormalization step starts to quickly dominate the computation completely, and thus for solving a high number of states it is critical to keep the total number of iterations at a minimum by using a high-order approximation for \mathcal{T} . However, since higher-order factorizations involve an increasing number of arithmetic operations, finite precision arithmetic poses limits on how high order expansions of type (4) are reasonable. As reported in the case of a separate implementation of ITP [4], we confirm that order 12 is usually the limit for double-precision arithmetic.

2.4. Including a homogeneous magnetic field

In the presence of a magnetic field \mathbf{B} characterized by a vector potential \mathbf{A} , the canonical momentum operator of an electron is, in SI-based Hartree atomic units,

$$\Pi = -i\nabla + \mathbf{A},$$

and the kinetic energy operator is $T = \frac{1}{2}\Pi^2$. This operator is no longer diagonal in wave vector space, so applying the operator $\exp(-\varepsilon T)$ is no longer trivial. However, as noted by Aichinger et al. [2], when the magnetic field is homogeneous and parallel to the z -axis, the required exponential term can be factorized *exactly*:

$$\begin{aligned} \exp(-\varepsilon T) &= \exp\left(-\frac{\varepsilon}{2}(\Pi_x^2 + \Pi_y^2 + \Pi_z^2)\right) \\ &= \exp\left(-\frac{\varepsilon}{2}f_x(\xi)\Pi_x^2\right) \exp\left(-\frac{\varepsilon}{2}f_y(\xi)\Pi_y^2\right) \\ &\quad \times \exp\left(-\frac{\varepsilon}{2}f_x(\xi)\Pi_x^2\right) \exp\left(-\frac{\varepsilon}{2}\Pi_z^2\right), \end{aligned} \quad (5)$$

where Π_x , Π_y and Π_z are the x -, y - and z -components of Π , respectively, and the coefficients f_x and f_y are

$$f_x(\xi) = \frac{\cosh(\xi) - 1}{\xi \sinh(\xi)} \quad \text{and} \quad f_y(\xi) = \frac{\sinh(\xi)}{\xi}, \quad (6)$$

given as a function of $\xi = \varepsilon B$.

The next step is choosing the gauge of the vector potential in a way that each of term in factorization (5) can be implemented efficiently. The linear gauge $\mathbf{A} = (-By, 0, 0)$, where B is the magnetic field strength, is a good choice, because then the components of Π are simply $\Pi_x = k_x - By$, $\Pi_y = k_y$, $\Pi_z = k_z$, in terms of the wave vector $\mathbf{k} = (k_x, k_y, k_z)$. This means that the factorized $\exp(-\varepsilon T)$ can be applied to a wave function by first Fourier transforming from the (x, y, z) basis to (k_x, y, k_z) , where both $\exp(-\frac{\varepsilon}{2}\Pi_z^2)$ and $\exp(-\frac{\varepsilon}{2}f_x(\xi)\Pi_x^2)$ are diagonal and easily applied. Then we can Fourier transform the remaining y -coordinate in order to get to the basis (k_x, k_y, k_z) where $\exp(-\frac{\varepsilon}{2}f_y(\xi)\Pi_y^2)$ is diagonal. Finally we transform back to (k_x, y, k_z) in order to apply $\exp(-\frac{\varepsilon}{2}f_x(\xi)\Pi_x^2)$ again. All steps require only Fourier transforms and pointwise multiplications, and moreover, the number of required Fourier transforms is not increased from the case of zero magnetic field.

This method of exact factorization of the kinetic energy part allows for a (possibly very strong) homogeneous external magnetic field to be included in ITP simulations without any additional approximations. Another attractive feature of this method is that it can be made gauge-invariant regardless of the discretization [3], removing gauge-origin problems that often affect computations with magnetic fields.

2.5. Treating Dirichlet boundary conditions

Throughout the previous discussion, the use of Fourier transforms to go from the position to the wave-vector basis has implied the use of periodic boundary conditions. Switching to Dirichlet boundary conditions would allow the study of billiard systems, which are common model systems in quantum chaos research [6].

A simple way to enforce Dirichlet boundary conditions for a rectangular calculation box is to replace the Fourier transforms with sine transforms, or in other words, to expand the wave functions in eigenstates of a particle in a rectangular box instead of plane waves. However, there are two complications in this simple approach. First of all, the use of the sine transform still implies periodicity across the boundary. The wave functions will be periodic because of the Dirichlet boundary conditions, but the wave functions can have a discontinuous derivative at the boundary. Because of this possible discontinuity of the derivative, the expansions in sine waves can have spurious, high-frequency “ringing” artifacts. These artifacts will be dampened by the ITP iterations, but they will worsen convergence.

Secondly, with an external magnetic field the sine waves are no longer as good a basis. For example, applying the Hamiltonian to a combination of sine functions results in a combination of sine and cosine functions, since with a magnetic field the Hamiltonian also includes first derivatives. Previously, operators such as the kinetic energy and the exponential of kinetic energy turned out to be simple: Fourier transform to the wave-vector space, a multiplication, and a transform back. With a magnetic field and Dirichlet boundary conditions they become a sine transform, two multiplications, and two inverse transforms, because the sine and cosine parts need to be handled separately. The correct basis to use would be the eigenfunctions of a particle in a rectangular box with a magnetic field, but to this problem no simple solution is known – computing these eigenfunctions was a major goal for *itp2d*, and the reason Dirichlet boundary conditions were implemented in the code.

It should be pointed out, however, that these problems do not prevent combining Dirichlet boundary conditions with an external magnetic field, they only cause slower converge. Our implementation can, for example, solve the first few thousand eigenstates of the particle in a box with a magnetic field. Improving the combination of Dirichlet boundary conditions and a magnetic field will be a major goal for future development of the code.

2.6. Convergence checking

As discussed previously, the ITP scheme with a fixed imaginary time step ε converges faster with larger ε , but to a more inaccurate solution. For this reason the ITP scheme is traditionally coupled with time step adjustment, i.e., the states are first converged with a larger time step and the time step is subsequently decreased, iterating this converge-decrease cycle until some final criteria of convergence is fulfilled. There are therefore two “levels” of convergence involved: convergence with respect to the current value of ε , and final convergence.

A natural measure of final convergence for a state ψ is the standard deviation of energy

$$\sigma_H(\psi) = \sqrt{\langle \psi | H^2 | \psi \rangle - \langle \psi | H | \psi \rangle^2},$$

where H is the system Hamiltonian. This quantity also gives an error estimate for the computed eigenenergies. Convergence with respect to the time step can be considered by looking at the change of σ_H between successive iterations – when the standard deviation no longer decreases by a significant amount between iterations, the state can be considered converged with the current time step.

Simpler measures of convergence can be implemented by looking directly at the values of energy obtained at each iteration and considering the state converged when either the relative or absolute change in energy between successive iterations gets small enough. Another simple way of defining final convergence is the point when decreasing the time step seems to be of no use, i.e., the point when after decreasing the time step, the state converges with respect to the decreased time step with only one iteration.

Due to the fact that the convergence checks represent in any case an insignificant share of the total computational resources, it is usually best to use the standard deviation as a measure of convergence. The simpler methods come to play only when something prevents the use of the standard deviation. This occurs, for example, when using an external magnetic field combined with the method of enforcing Dirichlet boundary conditions discussed in Section 2.5, since the ringing artifacts near the edges make the computation of $\langle \psi | H^2 | \psi \rangle$ inaccurate.

3. Implementation

3.1. Program structure overview

Our implementation of ITP for two-dimensional systems, *itp2d*, is based on a high-level, object-oriented design, with calls to optimized external routines for time-consuming low-level operations. This makes the program easier to maintain and extend without compromising computational efficiency. All computations are done in SI-based Hartree atomic units and for simplicity, Hartree atomic units are also used for all input and output (except timing data, which is given in seconds).

The complete ITP simulation implementation is encapsulated in a single high-level C++ class, making our program easily included in separate programs needing a fast Schrödinger equation solver, e.g., for solving the Kohn–Sham equations for density-functional theory calculations. This high-level C++ interface is supplemented with a simple (but complete) command line interface, that provides an easy way to run simulations with different parameters without recompiling. The command line interface is implemented using the Templated C++ Command Line Parser Library (TCLAP).

The program is distributed with a separate documentation file that covers the use of *itp2d* from a more practical point of view. The command line interface also includes inline documentation, accessible with the command line argument `--help`.

For compiling *itp2d* a simple GNU Makefile is provided. The Makefile is designed for the free and portable g++ compiler from

the GNU Compiler Collection. The actual program code in `itp2d` should be standards compliant C++, so other standards compliant compilers can also be used, but this requires modifications to the Makefile. In a similar way, `itp2d` is only tested on computers running Linux, but the program should work in other systems with minimal effort, provided a C++ compiler and the required external routines are available.

3.2. Implementation of the ITP scheme

The wave functions operated on by ITP are implemented as two-dimensional arrays of double precision complex numbers on a rectangular grid with uniform spacing. This low-level memory layout is supplemented with a high-level class interface providing the necessary arithmetic operations. Similar class interfaces are provided for arrays of wave functions for easily handling several wave functions as a whole. Operators acting on wave functions are similarly defined in an object-oriented fashion, with support for defining sums and products of operators with simple arithmetic operations.

The potential part of the Hamiltonian operator is implemented with direct pointwise multiplication of the wave function with precomputed values. A few common potential types are provided, and implementing new ones is as easy as providing a C++ routine which gives the values of the potential as a function of position. There is also rudimentary support for adding arbitrary types of random noise to the potentials.

In the case of periodic boundary conditions with no magnetic field the kinetic energy part of the Hamiltonian is implemented by simply expanding the wave function in plane waves via a discrete Fourier transform, multiplying with $\mathbf{k}^2/2$, where \mathbf{k} is the wave vector, and returning to the position basis via an inverse discrete Fourier transform. External magnetic field only shifts the eigenvalues of the momentum operator with the vector potential \mathbf{A} , so in the case of nonzero magnetic fields, the states simply need to be multiplied with $(\mathbf{k} + \mathbf{A})^2/2$. As discussed in Section 2.4, the magnetic field is assumed to be homogeneous and parallel to the calculation plane, and for numerical efficiency all wave functions and operators are expressed in the linear gauge $\mathbf{A} = (-By, 0, 0)$. For Dirichlet boundary conditions, states are expanded in eigenstates of the particle in a box (via a discrete sine transform). The kinetic energy operator with no magnetic field is again a simple multiplication in the sine function basis, but as discussed in Section 2.5, the case of nonzero magnetic field is more complicated. In this case the operator is split into two parts, $(-i\nabla + \mathbf{A})^2/2 = (-\nabla^2 + \mathbf{A}^2)/2 - i\mathbf{A} \cdot \nabla$, so that the first part is a simple multiplication in the sine function basis, and the second one turns the sine functions into cosines multiplied by a suitable factor, i.e., it is a sine transform followed by a multiplication and an inverse cosine transform.

The exponentiated operators $\exp(-\varepsilon V)$ and $\exp(-\varepsilon T)$ required for imaginary time propagation are implemented using Fourier or sine transforms in a similar way as the original potential and kinetic energy operators. The exponentiated potential operator is still a pointwise multiplication in the position basis, and as discussed in Section 2.4 the exponentiated kinetic energy operator can be factorized into parts that can be implemented with discrete Fourier transforms and pointwise multiplications. In both cases the multiplication arrays are precomputed and only recalculated when the time step ε is changed. The full imaginary time propagation operator is then built from the two operators by operator arithmetic as specified by the Chin factorization [1] given in Eq. (4), up to the order specified by the user. The resulting chain of operator sums and products is simplified when possible by absorbing constant prefactors into the operators themselves and combining adjacent multiplications.

The orthonormalization of wave functions is implemented using the Löwdin method described in Section 2.2. The inner products and the diagonalization of the overlap matrix are simply delegated to external linear algebra routines. For the linear combination two alternative algorithms are provided: the default one in which the large matrix product (2) is split into matrix-vector products in order to use as little extra memory as possible, and one where the product is calculated directly, requiring an extra copy of the wave functions. The latter algorithm may be faster in some cases since it makes maximal use of optimized external routines, but this is offset by the roughly double memory requirement which makes a huge difference for large systems.

The ITP cycle is started with random noise as the initial wave functions. This helps to ensure that no eigenstate of the Hamiltonian is missing from the expansions of the initial states due to accidental orthogonality, as discussed in Section 2.1. The desired number of states to be converged is provided by the user, as is the total number of states to be included in the computation. If the latter is missing, the program adds 25% to the number required to converge. This default value was empirically determined to provide a good convergence speed. The initial imaginary time step ε is also provided by the user, and after all the required states have converged with respect to the time step size, it is decreased by dividing by a user-provided constant. It is also possible to fine-tune the convergence by explicitly listing all time step values that are to be used. Each time convergence with respect to the time step is found, states are also tested against the criteria of final convergence, and if it is fulfilled by all the required states the computation ends. The criteria for convergence are also provided by the user. By default the program uses the standard deviation with respect to the Hamiltonian, but other criteria listed in Section 2.6 have also been implemented.

3.3. Data file output

In addition to the textual output given by the command-line interface, `itp2d` saves its results and parameters as portable HDF5 data files. All data coming from a single simulation run are saved in a single data file. The user can specify whether, in addition to the parameters given to the simulation, only final energies (along with their error estimates) are saved, or also the final wave functions, or even intermediate wave functions after each iteration. Using a common (as opposed to application-specific) data file format has several advantages. First of all, the data can be imported easily to common data analysis software, and accessing the data is easy: the HDF5 format presents the data as a directory of data sets, with descriptive names for each set. With HDF5 even complicated, multidimensional data can be saved without trouble and without complicating later data access.

3.4. Parallelization

Many parts of the ITP computation are suitable for shared-memory parallelization. The most trivial case is the actual propagation step, where each state is operated on by the imaginary time propagation operator independent of each other. In a similar way, the task calculating the energy and standard deviation of energy for each state is trivially split to several, independent processing threads. The orthonormalization step is not as easily parallelized, but most of the work can be distributed by calculating the inner products for the overlap matrix in parallel, and splitting the matrix product of Eq. (2) into matrix-vector products which are executed in parallel.

In all above cases our implementation uses high-level OpenMP instructions for parallelization, making the parallelized code simple and readable. It should be noted that due to the large

amount of data that needs to be passed to the execution threads, especially for parallelizing the orthonormalization step, ITP works best with shared-memory parallelization, i.e., several execution cores accessing the same physical memory. When using the program in large cluster computers special care should be taken to ensure that there is no unnecessary memory access across slow network links.

3.5. External routines

To avoid needless reimplementations, most low-level numerical operations used in `itp2d` are delegated to external routines. This also allows the user to use routines heavily optimized to the current hardware. All linear algebra routines are accessed via standard LAPACK and CBLAS interfaces. Our program has been tested with the portable ATLAS implementation, the MKL library from Intel, and the ACML library from AMD. Discrete Fourier, sine and cosine transformations are computed using the heavily optimized library FFTW3 [12]. Intel's MKL library provides a FFTW3-compliant interface, but using MKL for the transformations has not been tested with our program.

3.6. Provided unit tests

Our program is distributed with a comprehensive unit test suite, implemented with the Google C++ Testing Framework. The unit tests cover several low-level details, such as the accuracy of external Fourier transform routines and the internal logic of several arithmetic operations, and high-level features, such as running ITP simulations using potentials with known analytic eigenstates and comparing the results. It is advisable to always run this unit tests suite before important calculations to protect against unforeseen errors.

3.7. Open source

We release `itp2d` under an open-source license with the intention that it will foster wide use and future development of the code. Users are encouraged to improve and extend the code and share their changes with other users of `itp2d`. More information about getting involved can be found in the README file distributed with `itp2d`.

4. Numerical tests

4.1. The harmonic oscillator

The harmonic oscillator is an example of a system with a known analytic solution with or without a magnetic field. The harmonic oscillator with potential $V(\mathbf{r}) = \frac{1}{2}r^2$ is also the default potential used in `itp2d`, so simply running the program with no additional command line parameters will produce the first few eigenstates of the harmonic oscillator. The energy levels of the above potential will follow the Fock–Darwin spectrum

$$E_{nl}(B) = (2n + |l| + 1)\sqrt{1 + \frac{1}{4}B^2} - \frac{1}{2}lB, \quad (7)$$

with $n = 0, 1, 2, \dots$, $l = 0, \pm 1, \pm 2, \dots$

Table 1 collects some eigenenergies computed for the harmonic oscillator by `itp2d` from a simulation with 4000 states required to converge (5000 states in total) and magnetic field strength $B = 1$. The final convergence criteria used was a relative standard deviation of energy σ_H/E of less than 10^{-3} . As is seen in the table, the accuracy of computed energies is very good up to highly excited states, and in most cases σ_H gives a good upper bound estimate of

the actual error in the result. For state 1000 the standard deviation σ_H is less than the actual error. In general, very small values of σ_H are not reliable due to discretization errors. This simulation required 5 iterations of ITP starting with time step $\varepsilon = 0.1$. The simulation used a 500 by 500 grid and 12th order operator splitting.

4.2. High energy eigenstates of a particle in a box with a magnetic field

The particle in a box, i.e., a potential that is zero inside a rectangular box and infinite elsewhere, is another example of a potential with a known energy spectrum – except for the case with nonzero magnetic field. With a magnetic field the system is no longer trivial, and no analytic solution is known. Another interesting feature of this system is that the corresponding classical system shows chaotic behavior [13,14], making the particle in a box with magnetic field an interesting testbed for quantum chaos studies.

Since the system combines Dirichlet boundary conditions and a magnetic field, it is subject to the problems discussed in Section 2.5, i.e., slower convergence and inaccurate calculation of σ_H . However, in order to illustrate that these problems do not prevent the study of this system with `itp2d`, we demonstrate that we have calculated a thousand eigenstates of this system. However, since no analytic expression of the energy is known, and since we are not aware of any other program that could compute this many eigenstates of this particular system, assessing the accuracy of the calculation is difficult. The ITP calculation still converges, and the wave functions show no sign of numerical error. Due to the complicated interplay of the magnetic field and the “hard” potential walls, the eigenstate wave functions have a very intricate form, as shown in Fig. 1. The wave functions of a square billiard in magnetic field have been reported previously only for the first few eigenstates [15,16].

In our future studies we will focus on the chaotic properties of the present and other billiard systems in magnetic fields by examining the spectral properties in detail. The `itp2d` code is a versatile tool for that purpose.

4.3. Benchmark results

To assess the numerical efficiency of our program, we have benchmarked `itp2d` against publicly available general-purpose eigensolvers. The solvers used in our test were PRIMME [17] (version 1.1) and SLEPc [18] (version 3.3-p2), the latter also functioning as an interface for ARPACK (arpack-ng version 3.1.2). Our benchmark consisted of solving an increasing number of eigenstates of a quartic oscillator potential in zero magnetic field, and measuring the elapsed wall time. The computations were run without parallelization. The results of this test are shown in Fig. 2.

As with any benchmark, the results need to be interpreted with care. It is very difficult to compare the performance of different programs and different algorithms completely fairly. Besides `itp2d`, the tested eigensolvers only use the Hamiltonian of the system to compute the eigenstates. In this test all eigensolvers use the Hamiltonian implemented in `itp2d`, which provides `itp2d` with an advantage. The other solvers compute matrix-vector products of the Hamiltonian and a state vector out-of-place (i.e., without overwriting the original state), whereas the Hamiltonian implementation of `itp2d` is in-place. This incurs an overhead, since each matrix-vector product requires the vector to be copied. This overhead was measured to be small (a few percent of total runtime), and it was subsequently subtracted from the results shown in Fig. 2. Some advantage still remains from the fact that in-place Fourier transforms computed with

Table 1

Calculated energy levels of a harmonic oscillator potential $V(\mathbf{r}) = \frac{1}{2}r^2$ with magnetic field strength $B = 1$. The table also shows the standard deviation of energy σ_H , the exact value of energy, and the actual error of the result. All results are from a single simulation with 5000 states. The final convergence criteria was that the first 4000 states have $\sigma_H/E < 10^{-3}$. As is evident from the results, the lower energy states converge to a lot higher accuracy.

#	E	σ_H	E_{exact}	$ E - E_{\text{exact}} $
0	1.118033988749895	6×10^{-8}	1.118033988749895	$< 10^{-15}$
10	4.5901699437497	2×10^{-11}	4.590169943749475	3×10^{-13}
100	14.152475842500	4×10^{-11}	14.152475842498529	3×10^{-12}
400	28.311529493753	5×10^{-11}	28.31152949374527	9×10^{-12}
1000	44.74922359501	8×10^{-12}	44.74922359499622	3×10^{-11}
2000	63.25580140378	6×10^{-11}	63.25580140374443	4×10^{-11}
4000	89.4495	6×10^{-2}	89.44929690873981	3×10^{-4}

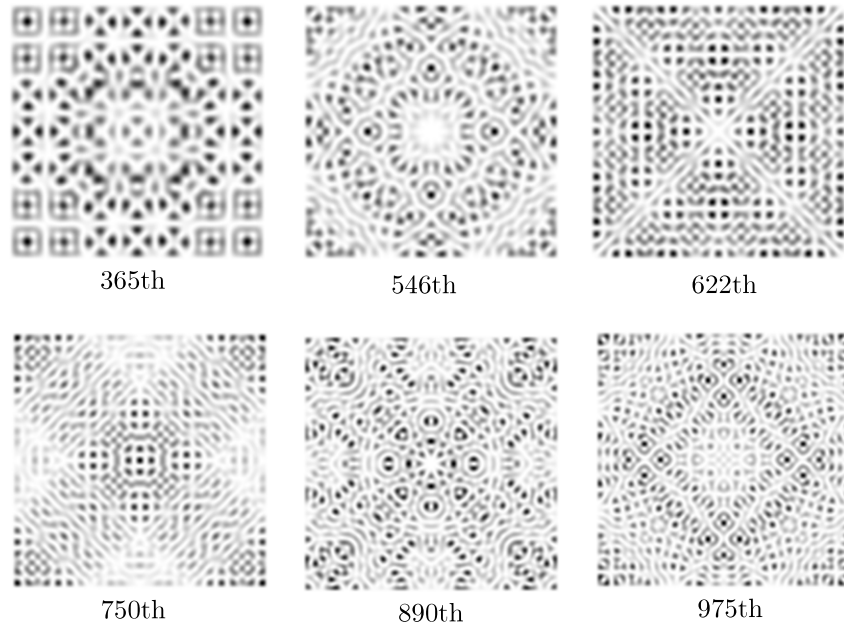


Fig. 1. Density plots of a few collected eigenstates of the particle in a box with a magnetic field. The eigenstates were calculated by *itp2d* for a π by π box with magnetic field strength $B = 1$.

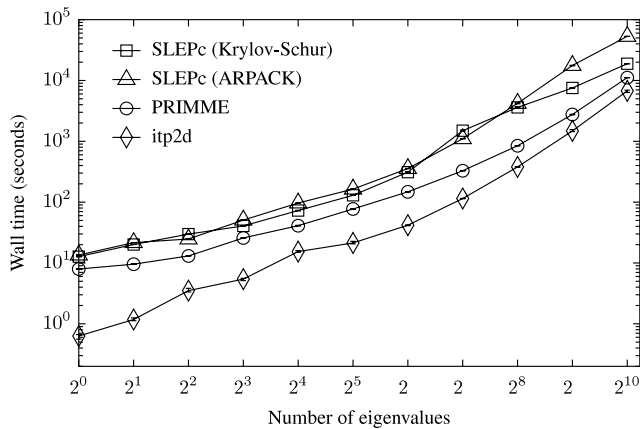


Fig. 2. Elapsed wall time in an eigenstate computation as a function of the number of eigenstates. The results are shown for four different solvers: SLEPc using its default solver algorithm (Krylov-Schur), SLEPc interface for ARPACK, PRIMME, which implements several solver algorithms and chooses the optimal one dynamically, and *itp2d*. All computations were repeated three times, and the average wall time was used for making the figure. The error bars on the data points show the minimum and maximum wall time value, respectively. The same Hamiltonian operator implementation, the same grid size and the same convergence criterion were used for all computations. The computations were done on a single, dedicated workstation.

FFTWF3 are somewhat slower than their out-of-place variants [12]. Another issue which complicates the interpretation of this simple

benchmark is that all the tested programs and algorithms have several parameters, and truly optimal performance would require fine-tuning these parameters for each system and problem size. For example, different preconditioning strategies were not tested for any of the contestants.

As a conclusion, even though our simple benchmark does not capture the whole truth regarding the performance of *itp2d* compared to other programs, we are confident that *itp2d* performs on a level which is comparable to other eigensolver implementations.

5. Summary

The program we have presented, *itp2d*, is a modern implementation of the imaginary time propagation algorithm for solving the single-particle, time-independent Schrödinger equation in two dimensions. Its strengths include a clear, object oriented design, and the ability to include a strong, homogeneous magnetic field. It is released with the aim of providing researchers with a flexible and extensible code package for solving the eigenstates and energy spectra of two-dimensional quantum systems.

As immediate applications, we find appealing possibilities in the field of quantum chaos in terms of spectral statistics. Furthermore, it is straightforward to combine *itp2d* with real-space electronic-structure methods based on density-functional theory, e.g., into the Octopus code package [19].

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References

- [1] S.A. Chin, *Celestial Mech. Dynam. Astronom.* 106 (2010) 391.
- [2] M. Aichinger, S. Chin, E. Krotscheck, *Comput. Phys. Commun.* 171 (2005) 197.
- [3] S. Janecek, E. Krotscheck, *Phys. Rev. B* 77 (2008) 245115.
- [4] S.A. Chin, S. Janecek, E. Krotscheck, *Comput. Phys. Commun.* 180 (2009) 1700.
- [5] S. Janecek, E. Krotscheck, *Comput. Phys. Commun.* 178 (2008) 835.
- [6] H.-J. Stöckmann, *Quantum Chaos: An Introduction*, Cambridge University Press, New York, 2006.
- [7] T. Betcke, *Numerical Computation of Eigenfunctions of Planar Regions*, Ph.D. Thesis, University of Oxford, 2005.
- [8] A.H. Barnett, A. Hassell, *SIAM J. Numer. Anal.* 49 (2011) 1046.
- [9] L. Lehtovaara, J. Toivanen, J. Eloranta, *J. Comput. Phys.* 221 (2007) 148.
- [10] P.-O. Löwdin, *J. Chem. Phys.* 18 (1950) 365.
- [11] B.C. Carlson, J.M. Keller, *Phys. Rev.* 105 (1957) 102.
- [12] M. Frigo, S.G. Johnson, *Proc. IEEE* 93 (2005) 216.
- [13] N. Berglund, H. Kunz, *J. Stat. Phys.* 83 (1996) 81.
- [14] M. Aichinger, S. Janecek, E. Räsänen, *Phys. Rev. E* 81 (2010) 016703.
- [15] M.A.M. de Aguiar, *Phys. Rev. E* 53 (1996) 4555.
- [16] R. Narevich, R.E. Prange, O. Zaitsev, *Phys. Rev. E* 62 (2000) 2046.
- [17] A. Stathopoulos, J.R. McCombs, *ACM Trans. Math. Software* 37 (2010) 21:1–21:30.
- [18] V. Hernandez, J.E. Roman, V. Vidal, *ACM Trans. Math. Software* 31 (2005) 351.
- [19] M.A.L. Marques, A. Castro, G.F. Bertsch, A. Rubio, *Comput. Phys. Commun.* 151 (2003) 60.