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

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We present our open-source code [1, 2] for solving the single-particle, time-independent Schrödinger equation in two dimensions. Our program, `itp2d`, utilizes the imaginary time propagation (ITP) algorithm, and it includes the most recent developments in the ITP method: the arbitrary order operator factorization [3] and the exact inclusion of a (possibly strong) external magnetic field [4]. In our implementation we emphasize a modern and easily extensible design, simple and user-friendly interfaces, and an open-source development philosophy. Our program is able to solve thousands of eigenstates of a two-dimensional quantum system in a reasonable time with commonly available hardware. The main motivation behind our work is to allow the study of highly excited states and statistical properties of energy levels of two-dimensional quantum dots and billiard systems with a single versatile code, e.g., in research on quantum chaos. Furthermore, `itp2d` can be combined with real-space electronic-structure methods based on, e.g., density-functional theory.

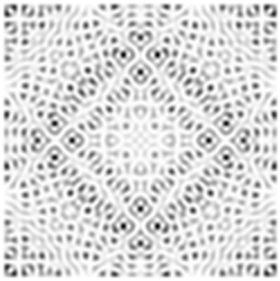

Figure 1: Density plot of the 975th eigenstate of a particle in a box with a strong external magnetic field.

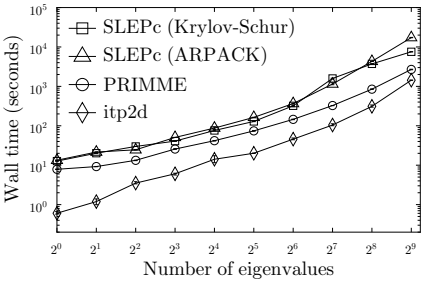

Figure 2: Elapsed wall time as a function of the number of solved eigenstates for four different programs, including our `itp2d`.

[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, S. A. Chin, E. Krotscheck, Comput. Phys. Commun. **171**, 197 (2005).