A fast explicit solver for Gross-Pitaevskii equation

Jeffrey M. Brown

April 15, 2016

1 Introduction

A fast explicit solver for the Gross-Pitaevskii equation (GPE) based on Visscher's method for time propagating Schrödinger's equation is demonstrated. Visscher's method was first published[1] in 1991, but still remains relatively unknown compared to alternative methods, such as Crank-Nicholson or the split-step method. Visscher's method has the advantage that it offers the same relative order of accuracy, but is faster running and much easier to code due to its simple update scheme. This makes it a good candidate for pedagogical demonstration of quantum system dynamics. In the following sections Visscher's method for the Schrödinger equation is explained, then the update scheme to include the nonlinear term found in GPE is modified and finally it is shown that the method reproduces some well known examples of Bose-Einstein condensate (BEC) time dynamics.

2 Visscher's Method

The method begins by separating the wavefunction into its real R and imaginary I components. Schrödinger's equation now becomes a set of coupled equations

$$\frac{dR}{dt} = \hat{H} I \tag{1}$$

$$\frac{dI}{dt} = -\hat{H} R \tag{2}$$

where the real part is updated by the Hamiltonian $\hat{H}$ acting on the imaginary part and vice versa. Visscher suggests that equations (1) and (2) are solved more easily by placing the real and imaginary parts at offset times. By approximating the time derivative with a simple finite difference and rearranging the equations, the update scheme becomes

$$R\left(t + \tfrac{1}{2}\Delta t\right) = R\left(t - \tfrac{1}{2}\Delta t\right) + \Delta t H I\left(t\right) \tag{3}$$

$$I\left(t + \tfrac{1}{2}\Delta t\right) = I\left(t - \tfrac{1}{2}\Delta t\right) - \Delta t H R\left(t\right) \tag{4}$$

[1] A fast explicit algorithm for the time-dependent Schrödinger equation, P.B. Visscher, Computers in Physics 5, 596 (1991); doi: 10.1063/1.168415

and the system evolves forward in time Δt by applying (3) and (4) sequentially. The time evolution of one part of the wavefunction is determined by its counterpart at an offset time, approximating wavefunction evolution.

Due to the temporal offset of the wavefunction components, it may not be clear how to represent the probability distribution or calculate an expectation value at a given time t. Visscher suggests that at the times corresponding to the real part

$$|\psi(t)|^2 = R\left(t\right)^2 + I\left(t + \tfrac{1}{2}\Delta t\right) I\left(t - \tfrac{1}{2}\Delta t\right) \tag{5}$$

and for the times corresponding to the imaginary part

$$|\psi(t)|^2 = R\left(t + \tfrac{1}{2}\Delta t\right) R\left(t - \tfrac{1}{2}\Delta t\right) + I\left(t\right)^2. \tag{6}$$

The only constraint for these choices of probability is that we recover the continuum equations $|\psi(t)|^2 = R(t)^2 + I(t)^2$ as $\Delta t \to 0$. Therefore the above equations are a reasonable choice.

The final piece needed is the initial conditions $R(0)$ and $I\left(\frac{1}{2}\Delta t\right)$. If there exists an explicit formula for the time dependent wavefunction, then there is no problem in creating these initial conditions. However, in most cases the time dependent nature of the initial wavefunction is not known, such as a numerically computed ground state of a particular potential. Visscher's method has the extra burden of knowing the real and imaginary parts of the initial wavefunction at different times. A similar problem exists for initializing the electric and magnetic fields in a finite difference Maxwell solver. This of course does not prevent this scheme from being useful, but care must be taken when providing a accurate initial conditions.

One final note on the temporal offset of the wavefunction's real and imaginary components: Visscher's method loses its fast explicit scheme (and becomes an implicit method) if the system is propagated in complex-valued time. Since propagating in complex-valued time is a common method for finding the ground state of a given potential, it is recommended that a spectral method (or similar) is used for this task. Once the ground state is found, the update scheme can then be changed to Visscher's to evolve the system normally. Note that solving for the ground state for a particular potential is a one-time simulation, therefore this limitation is not a significant disadvantage.

3 Adaptation for GPE

Visscher's basic scheme must be modified in order to handle the nonlinear term present in GPE. For the Schrödinger equation, the update scheme is written explicitly as

$$R\left(t + \tfrac{1}{2}\Delta t\right) = R\left(t - \tfrac{1}{2}\Delta t\right) + \Delta t\left(-\tfrac{1}{2}\nabla^2 + V\right) I\left(t\right) \tag{7}$$

$$I\left(t + \tfrac{1}{2}\Delta t\right) = I\left(t - \tfrac{1}{2}\Delta t\right) - \Delta t\left(-\tfrac{1}{2}\nabla^2 + V\right) R\left(t\right) \tag{8}$$

where the laplacian is approximated at a point in a discrete array for the 1D case as $\nabla^2 f[x_i] = (f[x_{i-1}] + f[x_{i+1}] - 2f[x_i])/\Delta x^2$ and for the 2D case $\nabla^2 f[x_i, y_i] = (f[x_{i-1}, y] + f[x_{i+1}, y] + f[x, y_{i+1}] + f[x, y_{i-1}] - 4f[x_i, y_i])/\Delta x^2$. The scheme is explicit since the future values of R and I only depend on quantities that were calculated in the past. By adding in the nonlinear term $\eta|\psi(t)|^2$ for the appropriate time, the explicitness appears to be lost.

$$R\left(t+\tfrac{1}{2}\Delta t\right) = R\left(t-\tfrac{1}{2}\Delta t\right) + \Delta t\left(-\tfrac{1}{2}\nabla^2 + V + \eta\left[R\left(t+\tfrac{1}{2}\Delta t\right)R\left(t-\tfrac{1}{2}\Delta t\right) + I\left(t\right)\right]\right)I\left(t\right) \tag{9}$$

$$I\left(t+\tfrac{1}{2}\Delta t\right) = I\left(t-\tfrac{1}{2}\Delta t\right) - \Delta t\left(-\tfrac{1}{2}\nabla^2 + V + \eta\left[R(t) + I\left(t+\tfrac{1}{2}\Delta t\right)I\left(t-\tfrac{1}{2}\Delta t\right)\right]\right)R\left(t\right) \tag{10}$$

Luckily, the equations are still linear allowing $R(t+\frac{1}{2}\Delta t)$ and $I(t+\frac{1}{2}\Delta t)$ to be solved as

$$R\left(t+\tfrac{1}{2}\Delta t\right) = \frac{R\left(t-\frac{1}{2}\Delta t\right) + \Delta t\left[-\frac{1}{2}\nabla^2 + V + \eta I(t)^2\right]I\left(t\right)}{1 - \Delta t\eta R\left(t-\frac{1}{2}\Delta t\right)I\left(t\right)} \tag{11}$$

$$I\left(t+\tfrac{1}{2}\Delta t\right) = \frac{I\left(t-\frac{1}{2}\Delta t\right) - \Delta t\left[-\frac{1}{2}\nabla^2 + V + \eta R(t)^2\right]R\left(t\right)}{1 + \Delta t\eta R\left(t-\frac{1}{2}\Delta t\right)I\left(t\right)}. \tag{12}$$

This update scheme that takes into account the nonlinearity in GPE and fortunately the LHS values are calculated from only past values, therefore no iterative methods are needed. A quick sanity check shows that Visscher's update scheme for the Schrödinger equation is recovered as $\eta \to 0$. These update equations are only slightly more complicated that the original ones and should provide a fast update scheme to model the time evolution of a BEC.

The next questions to address is how small should the time step be for a given spatial discretization? A rough estimate of the stability criterion for this algorithm can be estimated using the criterion in Visscher's paper, which is $\Delta t < \Delta x^2$. This criterion assumes that the value of the potential $V = 0$ and ignores the effects of nonlinearity. This of course is an upper bound for Δt, therefore in practice $\Delta t < \frac{1}{4}\Delta x^2$ seems to be a reasonable choice for the types of potentials and strengths of nonlinearity found in BEC systems. Deriving a more rigorous criterion equation is impractical due to the nonlinear term in GPE, since it would require knowing the max value of $|\psi|^2$ for all times in the simulation. Therefore it's impossible to know whether a set of parameters would produce a stable evolution a priori. Luckily when the simulation becomes unstable, the wavefunction values grow extremely fast in magnitude and quickly produce NaN values. A simple periodic check could be implemented to check for NaN's, then halt the time evolution, and restart with a new smaller step size.

4 Results

To show that the update scheme works, some well-known BEC system dynamics are demonstrated. The first check is that as the nonlinearity is turned off $\eta = 0$,

then Visscher's update scheme for the Schrödinger equation is recovered. The exact solutions for a harmonic potential $V = \frac{1}{2}x^2$ are the well-known quantum harmonic oscillator (QHO) states $\psi_n(x,t) = \exp[-\frac{1}{2}x^2 - iE_nt]H_n(x)/\sqrt{2^n n!\pi^{1/4}}$. Figure 1 shows that the ground state wavefunction ($n = 0$ and $E_0 = 0.5$) remains stationary after propagating 10 atomic units of time. This is just a simple check of our code to make sure that it is accurately reproducing the linear part of GPE.

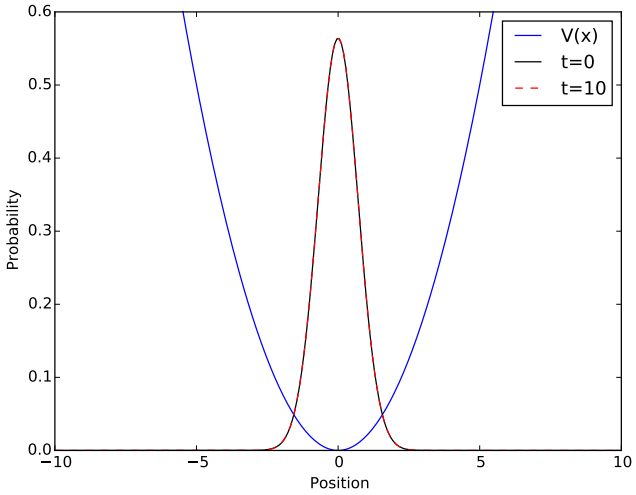

Figure 1: Quantum harmonic oscillator solution

To check that the nonlinear portion of GPE is reproduced accurately, another exact solution can be used. For the case of 1D and the potential $V = 0$, the GPE becomes the nonlinear Schrödinger equation and therefore has a stationary solution of $\psi(x,t) = \frac{1}{\sqrt{2}}\text{sech}(x)\exp(-i\mu t)$ with energy $\mu = -\frac{1}{2}$ for a nonlinearity of $\eta = -2$. Figure 2 shows that if the BEC wavefunction is initialized with the *sech* equation and evolve 10 atomic units of time forward, the wavefunction is unchanged. These two test demonstrate that the method has been coded correctly, and that the update scheme is stable and accurately reproduces known exact solutions for the given time step.

Now a test of a quasi-2D BEC for which an exact wavefunction solution does not exists is presented. The same QHO initial condition is used, but the nonlinearity value is changed to $\eta = 4$. Since this wavefunction is not a stationary state of the potential, some periodic behavior (similar to Section 4.2.4 of the class notes) should be seen. Since the harmonic trap and initial condition are radially symmetric, the BEC has periodic "breathing" as demonstrated in Figure 3.

For the final demonstration of the method, a vortex is embedded into the numerically calculated ground state wavefunction of a quasi-2D BEC. First, a spectral method is used to evolve an arbitrary wavefunction in complex-valued

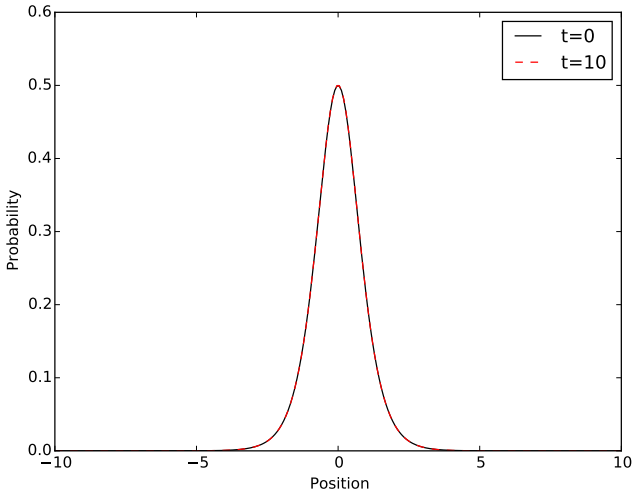

Figure 2: Sech(x) soliton solution for 1D GPE

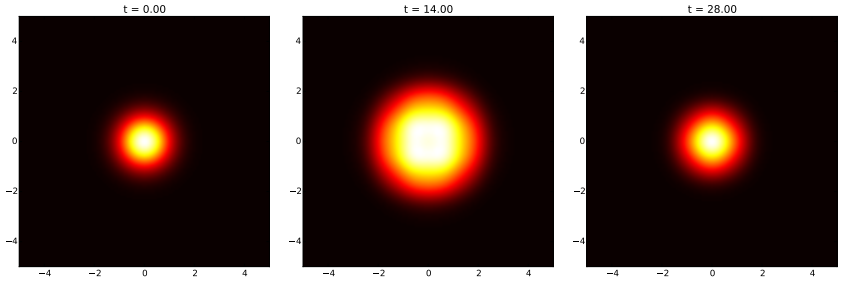

Figure 3: Breathing mode

time, where it decays to the ground state of a harmonic trap with a nonlinearity of $\eta = 4$. Within this wavefunction, a phase singularity is placed (using equation (4.122) in Section 4.3.1 of the class notes). It is expected from the theory that the vortex will precess around the outer boundary and indeed it does, as shown in Figure 4. Changing the phase of the singularity to opposite charge results in the vortex changing its direction of precession.

It is clear that the newly developed method reproduces known BEC phenomena, but is it actually faster than the split step method? Figure 5 shows that the modified Visscher's method for GPE results in lower execution times compared to the split step method. This due to the computational complexity of the underlying update scheme. The most computationally intensive part of the split step method's update scheme is the Fourier transform. The 1D FFT algorithm scales as $\mathcal{O}(N \log_2 N)$ for a vector of length N, whereas the 1D discrete laplacian scales as $\mathcal{O}(N)$. For larger grids Visscher's method will have

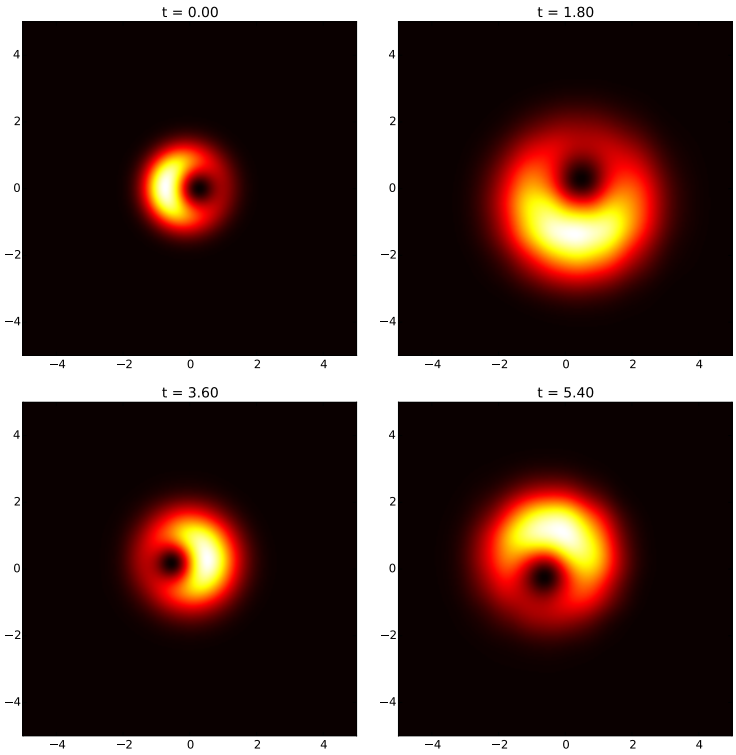

Figure 4: A vortex inside a quasi-2D BEC precesses around the perimeter.

drastically reduced runtimes. In Figure 5, the runtimes for a Python implementation of the split step method and Visscher's method for GPE is presented. The Python code suffers from garbage collection issues due to the temporary arrays being generated and removed during the update (most interpreted languages will have the same issues). This can be seen by the slight variation away from quadratic (an increase in runtime) around 1000 grid points, where the temporary arrays no longer fit into the smallest CPU cache. A C++ implementation of Visscher's method for GPE is also plotted for comparison. It does not have any temporary arrays and therefore plays nice with the CPU's caches. Regardless of the implementation, the numerical method developed here allows for larger grid simulations that can produce interesting results that run within the attention span of students.

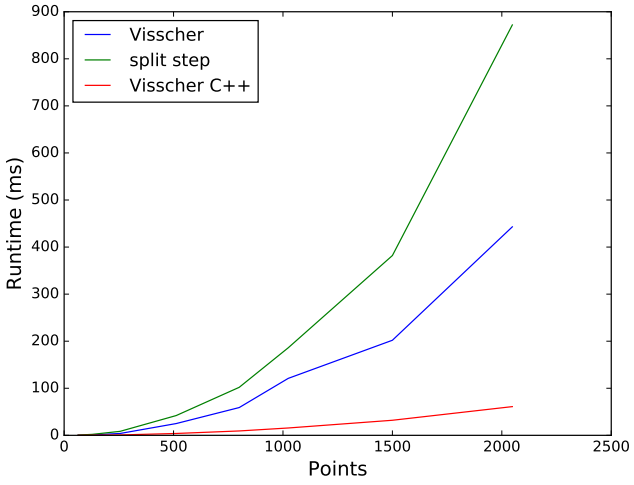

Figure 5: Plotted here is the time taking to make a single nonlinear step forward in time for a 2D grid with number of points along a side of N (total number of points in the grid is N^2). The method developed here scales better the than split step method using FFT.

5 Remarks

A fast and explicit time evolution scheme for modeling BEC dynamics has been demonstrated. The scheme reproduces many of the well-known examples and is relatively simple to implement, making it ideal for pedagogical purposes. The scheme does have one disadvantage in that the initial conditions require the real and imaginary parts of the wavefunction to be known at offset times. Another disadvantage is that there is not a straightforward way to evolve in complex-valued time, which is useful for numerically computing the ground states of arbitrary potentials. This is due to the nonlinear term $|\psi|^2$ and its definition of probability at time t that mixes real and imaginary components. These factors produce an implicit nonlinear update scheme when $H \to (1-\alpha)H$. One possible way around this, without resorting to the split step method, would be to extrapolate the offending term (something simple like $|\psi(t)^2| = 2|\psi(t-\Delta t)|^2 - |\psi(t-2\Delta t)|^2$) from previous values by storing a few past wavefunctions. This is probably robust enough to stay stable, but these types of improvements start to overshadow the simplicity of the current method. The most pragmatic solution is to use the spectral method to find the ground state for a given set of input parameters once and save the resulting wavefunction to a file. Then subsequent exploration can begin with this initial condition and proceed with the fast method demonstrated here.