Two Algorithms for Numerical Simulation of Counter Propagating Matter Waves In Optical Lattices

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Abstract: - In this paper a combined algorithm for simulation of counter propagating matter waves in optical lattices is presented. The mathematical model is based on an adaptation of a similar steady state model previously used for beams propagation in photonic lattices. Using the same mathematical model we developed two different algorithms. The first one is focused on calculation speed and calculation of the final result. The second implementation is used to show the evolution of this process during propagation. We show shortcomings of each approach and advantages of their combined use.

Key-Words: - Simulation, Modeling, Numerical algorithms, Counter propagating waves

1 Introduction

Numerical simulations are often used for investigation of physical phenomena. Two versions of algorithm for simulation of counter propagating matter waves in optical lattices are presented.

In a dilute boson gas at sufficiently low temperatures particles can condense and, in this way, form a Bose–Einstein condensate (BEC). Since 1995, when this phenomenon was first observed [1, 2], BECs have gained much attention, due to the fact that these condensates can be precisely manipulated in experiment [3, 4]. On the other hand, properties of BECs show similarities with the physical systems studied in other branches of physics, such as nonlinear (NL) optics and NL wave theory. Similarities between these theories manifest themselves in dynamical equations used to describe the corresponding physical systems. More concretely, these theories share as their determining part the general NL Schrödinger equation (NLSE). In literature, there are several forms of NLSEs, and what they have in common is the term representing the nonlinearity. Within the mean-field model, the evolution of BECs is, in a pretty accurate way, described by the Gross–Pitaevskii equation (GPE). The NL term in this partial differential equation reflects the interatomic interaction in a diluted cold gas.

Numerical solutions of similar problems with NLSE have been solved using finite difference [5], finite element [6] and multi-configuration time-dependent Hartree-Fock method [7]. Simulation of BEC dynamics has also been implemented using multi processor machines [8]. In this paper we present implementation details of numerical simulation for interaction of two counter propagating (CP) condensates that are initially confined to the so-called pancake shape [9] and propagate head-on along the square optical lattice. Similar to the case of light beams propagating in photonic lattices we are interested in stable structures. Finding these structures is possible by using an adaptation of the steady state model based on beam-step propagation method. Solving of Gross-Pitaevskii equation can also be done using techniques that preserve certain intrinsic properties of the equation [10]. This approach is computationally very efficient but it does not simulate the process, it just gives the final state (solution). In other words, steps in the algorithm do not represent different steps in propagation but just iterations in the solution solving method. When simulating this process it is necessary to use 2+1 dimensions, which greatly increases calculation time and space. In our simulation we implement this 2+1 dimensional model, but optimized it by exclusion of unnecessary calculations.

The paper is organized as follows. In the next section we present the mathematical model for our simulations. In the third section we compare the

steady state and the time dependent method. In Section 4 we introduce our optimization and show results.

2 Mathematical Model

We study the interaction of two counter propagating (CP) condensates that are initially confined to the so-called pancake shape [9] and propagate head-on along the square optical lattice. In this manner we numerically consider the evolution of two BECs for which it is possible to take separated wave functions.

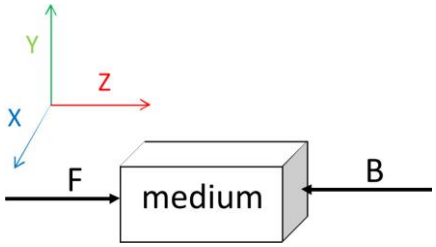

Figure 1. Problem geometry with forward (F) backword (B) BEC

The propagation of the forward (F) and the backward (B) BEC takes place in the longitudinal *z* direction, while we study the intensity in *(x,y)* plane. This propagation can be represented in by two coupled GPEs (Eq. 1):

$$\begin{aligned} -i\partial_z F &= \Delta F - VF - IF \\ i\partial_z B &= \Delta B - VB - IB \end{aligned} \tag{1}$$

where *F* and *B* are the forward and the backward wave functions, *I* is the total intensity of beams |F| and $|B|(|I|^2=|F|^2+|B|^2)$, *V(x,y)* is external potential. When simulating counter propagation we need to solve these equations. Δ is the transverse laplacian. We use the split-step (Fourier) method. The equation for each condensate is split into a pair of equations.

$$\begin{aligned} i\partial_z F &= \Delta F \\ -i\partial_z B &= \Delta B \end{aligned} \tag{2}$$

$$\begin{aligned} -i\partial_z F &= -VF - IF \\ i\partial_z B &= -VB - IB \end{aligned} \tag{3}$$

We solve the Eq. 2 in inverse space using Fast Fourier Transform

$$q^2 = k_x^2 + k_y^2 \tag{4}$$

$$\tilde{F}(z+dz,q) = e^{-iq^2 dz}\tilde{F}(z,q) \tag{5}$$

$$\tilde{B}(z-dz,q) = e^{-iq^2 dz}\tilde{B}(z,q) \tag{6}$$

In Equations 4,5 ~ is used to indicate function in inverse space. *dz* is the step size in *z* dimension. We use these solutions for the second pair of equations and their solution is

$$\begin{aligned} F(z+dz,\rho) &= e^{i(V+I)dz}F(z,\rho) \\ B(z-dz,\rho) &= e^{i(V+I)dz}B(z,\rho) \end{aligned} \tag{7}$$

These two steps combined give the solution of Eq. 1.

3 Implementation Details

When simulating the counter propagating BEC we have to define values of several parameters to fully define the process. First the dimensions of the problem in *x*, *y* dimensions and also the initial distance between the condensates *zmax*. Corresponding to these values, we define the number of greed points on each dimension *nxy*, *nz*. The number of grid points has to be selected in a fashion that the FFT procedure is correct. Potential *V* in our case was the following function:

$$V = V_0 \sin^2\left[\pi(x+y)/d\sqrt{2}\right]\times \sin^2\left[\pi(x-y)/d\sqrt{2}\right] \tag{8}$$

The last needed parameters are the initial values for forward F_0 and backward B_{nz} condensates.

We simulate the propagation of *F* from point 0 to *zmax* which corresponds to grid slice 0 to *nz* and the propagation of *B* in the opposite direction. In the initial approach we used the adaptation of the steady state model based on beam-step propagation method which is used for finding the final state. The implementation of this model (AL1) corresponds to the following pseudo code

do{
  $F^*=F_0$; $B^*=B_{nz}$
  $I_p = I_{nz/2}$
  $I_i^{*} = I_i^{*'}$
  for(i=0; i < nz ; i++){
    $F^* = FS_2\,(FS_1(F^*, I_i^*))$
    $I_i^{*'} = |F^*|^2$
  }
  for(i= nz-1; i >=0 ; i++){
    $B^* = BS_2\,(BS_1(B^*, I^*_{zn-i}))$
    $I_i^{*'} \mathrel{+}= |B^*|^2$
  }
} **while**($|I_{nz/2} - I_p| < \varepsilon$)

In pseudo codes for both algorithms we use FS_1, BS_1 for a function that calculate solutions for Eq. (5 , 6) and FS_2, BS_2 for Eq. 7. We first notice that in this algorithm the main loop is finished when the change in $I = |F|^2+|B|^2$ at the middle of the maximal distance has fallen below some test value ε. We chose *nz/2* for the test position due to the fact that the change in condensate energies is greatest at this position. In each iteration of the main loop we propagate condensates individually using 2D variables F^*, B^* over the whole distance between initial positions of condensates. We save the values of *I* in a 3D array which is used in the next step of the main loop. The connection between the two condensates is done only through *I*.

The algorithm basically works in the following way. At first step each condensate propagates without any interaction with the second one. In the following iterations, condensate propagation is computed more precisely with the previous value of I^* and a corrected value of $I^{*'}$ is prepared for the next step. The main advantage of this approach is fast convergence to solutions if they exist.

In our research we wanted to observe the evolution of this process. We implemented simultaneous propagation of condensates, and compared the results. We used the following algorithm (AL2)

```
for(j=0; j < nz ; j++ )
      for(i=1; i < j ; i++ ){
            I_i = |F_i|^2 +|B_i|^2
             F_i= FS_2 (FS_1(F_i-1,I_i))
            B_i= BS_2 (BS_1(B_zn-i+1_,I_i))
           }
}
```

In the second algorithm the outer loop finishes when both condensates have propagated the whole distance. Opposite to the approach in AL1 the interaction is calculated at each propagation step of *z* using the current value of condensates. To accomplish this we use two 3D arrays for storing the values of *F* and *B* over the entire propagation area. The inner loop simulates the propagation of the condensates for one step in the *z* direction. The movement of condensate *F* (*B*) for one grid block in *z* direction actually means that all known (previously calculated) sections move one step ahead. Their movement is affected by both, the section of the same condensate that is in front of them and the section of the counter propagating condensate at that position. With this algorithm both these effects have been taken into account.

For visualization of our results we use a different approach than proposed by Peter M. Ketcham and David L. Feder [11]. The goal of our simulation was to observe the effect of interacting condensates. We used a simpler method of visualization in which we excluded the information about the angular momentum. We have done this because we believed that images combining this information belonging to different condensates would have become cluttered and confusing. In our visualization we observe only the intensity of condensates, by creating isosurfaces for points having the same intensity for each of BEC separately. We color one of them in red and the other one in blue. In Fig. 2, 3 we show frames from animation created by this simulation.

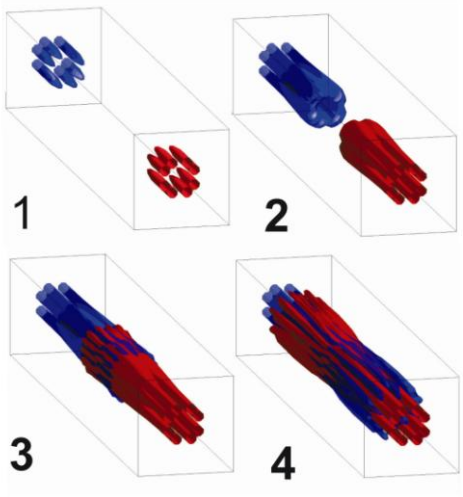

Figure 2. Simulation of interaction of the off-site CP solitons during propagation.

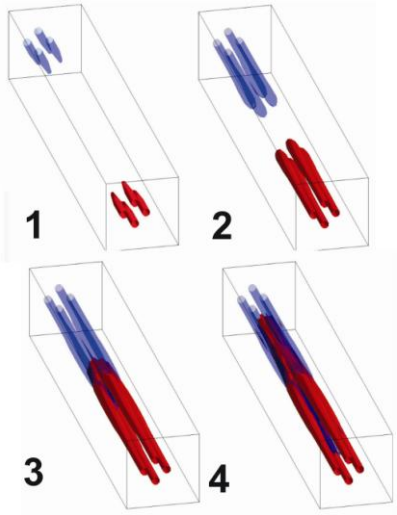

Figure 3. Simulation of interaction of the on-site CP solitons during propagation.

4 Comparison of Algorithms

Both of the algorithms for simulating BEC propagation have been developed using the same mathematical model and because of that it is necessary for final results to be equivalent to a certain level of precision. In our test this was confirmed.

We first consider the needed memory for implementing these algorithms. The memory was equivalent for both cases. In the first algorithm we needed two arrays of dimensions $nxy^2 * nz$ for storing the current values of I^*, and from the previous step $I^{*'}$. In the case of the second algorithm we needed two arrays of the same dimensions for storing F^*, B^*.

An exact comparisson of speed for these two models was not possible. In the case of the AL1 the number of iterations needed to achieve the desired precision for a certain problem size was not fixed and depended on potential V and initial values F_0, B_0, while in the other algorithm the number of iterations was only dependent of nz. In simulations that we performed the steady state algorithm was 2-5 times faster. The increase in calculation time was significant when we compare AL1 to AL2, but less than expected. This is due to the fact in the steady state case there is a smaller number in of iterations of the main loop, but all of them calculate zn steps for each of the condensates. Contrary to this, in the AL2 the number of steps for condensates grows as they propagate further. The relationship between calculation times was the following

$$AL1 : AL2 = \Pr ecisionIterations : \frac{zn}{2} \qquad (9)$$

To be able to observe properties of BEC propagation, the simulation had to be done with a high number of grid points. For x, y dimensions we used 1024 or 2048 and the number of grid point in the z dimension would be dependent on $zmax$ in the sense that the FFT procedure need to be correct. This resulted in long calculation time for which the increase of 2-5 times was in some cases unacceptable, and excluded the use of AL2.

One of the problems with AL1 is that the intermediate steps of the algorithm do not present relevant states of condensates, just their state in the iterative process. This is due to the fact that the algorithm starts with an unphysical state of condensates propagated next to each other without any effect on each other and it later corrects these values. A consequence of this is that until the desired precision is achieved, or in other words the algorithm finishes, we do not know if we have a valid physical state or not. Opposite to this, in the case of AL2 each step in the algorithm is physically valid and can be stopped at any desired moment in the case the process goes in an undesired direction. This gave us a more effective way to analyze the parameters of our simulation. An example would be the possibility of observing the maximal distance between condensates at which their interaction was relevant.

5 Conclusion

In this paper we have presented a simulation of propagating matter waves in optical lattices. The mathematical modeling for the problem was an adaptation of the steady state model that was previously used for light beams propagating in photonic lattices. We have shown the mathematical details of this model and details of the iterative method used for simulating propagation.

Using this mathematical model we implemented two different algorithms for simulating the BEC propagation. One that is optimized for finding final state (solution). The other algorithm is used to observe the evolution of the process. We have compared the properties of these two algorithms. As expected both algorithms gave the same final solutions, but differed in intermediate solutions. We have analyzed the memory requirements and speed for each simulation method. We have concluded that none of the two approaches can be considered as the superior one, but it depends what was the goal of the simulation. In practical use we realized that the best research method was the combined use of both algorithms. The use of simulation software using these algorithms resulted in publishing a paper in a physics journal [12].

Similar algorithms can be developed for other processes that can be modeled by NLSE. We believe that our analysis can be applied to them.

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