Handbook: 2D Gross-Pitaevskii Equation Solver

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1 Introduction

These notes detail the technical set-up of numerically solving the Gross-Pitaevskii equation based on the Crank-Nicolson method. No details will be given of the physical origin of the Gross-Pitaevskii equation; such information can be found in Ref. [1] .

We envisage a Bose-Einstein condensate or a more general superfluid composed of atoms. The system is parameterised by a wavefunction, $\psi(\mathbf{r},t)$. This wavefunction is complex and can be re-written in terms of a modulus and exponential phase factor,

$$\psi(\mathbf{r},t) = \sqrt{n(\mathbf{r},t)}\exp\left[i\theta\left(\mathbf{r},t\right)\right], \tag{1}$$

where $\theta(\mathbf{r},t)$ represents the phase and $n(\mathbf{r},t)$ is the atomic density (both of which are real quantities).

The wavefunction $\psi(\mathbf{r},t)$ is governed by the time-dependent Gross-Pitaevskii equation (GPE),

$$\mathrm{i}\hbar\frac{\partial}{\partial t}\psi(\mathbf{r},t) = \left(-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r},t) + g|\psi(\mathbf{r},t)|^2 - \mu\right)\psi(\mathbf{r},t) \tag{2}$$

Here m is the atomic mass, $V(\mathbf{r},t)$ represents the external potential acting upon the condensate (which may, in general, depend on time and position), g is the nonlinear coefficient (a constant) and μ is the chemical potential (another constant)[1].

2 The 2D GPE and its Dimensionless Form

2.1 Effective 2D systems and the 2D GPE

Imagine a 3D condensate where the wavefunction remains uniform in one direction, say the z direction. Such a picture is valid for lam-

[1] More often than not, the GPE will be written without the chemical potential appearing. Its inclusion in the GPE Hamiltonian causes a shift in the energy of the system, a permissible act since only changes in energy are physically relevant. We introduce it as it allows us to define the energy scale of the condensate, which comes in useful for normalizing the system, as we shall see.

inar flow and/or condensates which are so tightly confined in the z direction that motion is effectively prevented in that direction, e.g. a thin film or a quasi-2D trapped condensate. Then it becomes meaningful to consider a two-dimensional (2D) wavefunction $\psi(x, y, t)$. The corresponding density $n(x, y, t) = |\psi(x, y, t)|^2$ equates to the number of atoms per unit area (in the $x - y$ plane).

We can write the GPE in the corresponding 2D form (2D GPE),

$$\mathrm{i}\hbar\frac{\partial}{\partial t}\psi(x, y, t) = \left[-\frac{\hbar^2}{2m}\nabla^2 + V(x, y, t) + g|\psi(x, y, t)|^2 - \mu\right]\psi(x, y, t), \tag{3}$$

where the Laplacian operator becomes $\nabla^2 = \partial^2/\partial x^2 + \partial^2/\partial y^2$. These notes are concerned with numerically solving this 2D GPE in time and position.

2.2 Dimensionless form of the GPE

We may proceed to solve the GPE as it appears above. However, notice that the numbers involved in this equation are cumbersome, e.g. involving $\hbar$'s (of the order of 10^{-34}) and m's (of the order of 10^{-26}). We may put this equation into a more manageable form by rescaling the key quantities involved in the GPE using appropriately chosen units. This also has the benefit of making the results more generally applicable.

There are various ways to reduce the GPE to a dimensionless form. We choose a reduction where the units are based on those representing a homogeneous, infinitely-extended condensate. These units are often called *natural units*. Another common type of reduction is that of *harmonic oscillator units*, which is formulated based on a condensate confined by a harmonic-shaped trapping potential. The choice of units does not affect the remit of dynamics that can be studied, it is simply a choice of units to abide by. However, it can be more convenient to choose a set of units which most closely matches the physical system under study, e.g. harmonic oscillator units when modelling harmonically-trapped systems.

As our unit of density, we take the *peak density*, denoted n_0, which is the density in the absence of any potentials or excitations.

We take the *healing length*, denoted ξ (pronounced "si"), as our unit of length. The healing length is an important lengthscale in a condensate, e.g., setting the size of vortex cores, and is given by,

$$\xi = \frac{\hbar}{\sqrt{mn_0 g}}.$$

We take the *speed of sound*, denoted c, as our unit of speed. It is given by,

$$c = \sqrt{\frac{n_0 g}{m}}.$$

We take the chemical potential, denoted μ (pronounced "myu"), as our unit of energy. The chemical potential is expressed as,

$$\mu = n_0 g$$

Since $time = length/speed$ we can use the healing length and speed of sound to define a unit of time of ξ/c.

We will rescale the quantities in the GPE using these units, in other words we define,

$$x = x'\xi \qquad y = y'\xi \qquad t = t'(\xi/c) \qquad V = V'\mu \qquad \psi = \psi'\sqrt{n_0}$$

The primed variables will be our new *dimensionless* quantities.

Substituting these relations into the 2D GPE and cancelling common terms, we arrive at with the *dimensionless 2D GPE*:

$$i\frac{\partial \psi'}{\partial t'} = \left[-\frac{1}{2}\left(\frac{\partial^2}{\partial x'^2} + \frac{\partial^2}{\partial y'^2}\right) + V' + |\psi'|^2 - 1\right]\psi' \tag{4}$$

where $\psi' \equiv \psi'(x', y', t')$ and $V' \equiv V'(x', y', t')$. The cumbersome quantities have been removed from the equation, which is now more convenient and general. From now, we will deal solely with this dimensionless representation. For simplicity we henceforth drop the primes.

Under this dimensionless form, the energy of the condensate is of the order of unity. As a rule of thumb, this means that if we apply a potential with amplitude of 1 to some region of the system, the density will be just reduced to zero, i.e. all particles are removed from this region. As we decrease the size of the potential towards zero, the density in the region will increase, and when the potential becomes zero, the density should reach its unperturbed value of 1.

EXERCISE: Confirm that the GPE does indeed reduce to the dimensionless form shown in Equation (4) upon introducing the above dimensionless quantities.

3 Evolving the Wavefunction via Cayley's Approximation

Here we begin to detail the collection of numerical methods and procedures which enable us to computationally solve the 2D GPE. These are based on the notion of discretizing the wavefunction in time and space and operating on the wavefunction to evolve it to the next time step. The overall methodology is known as the Crank-Nicolson method.

3.1 Time-independent Hamiltonian

For the moment, let us assume the potential is not time-dependent, i.e. $V(\mathbf{r},t) \equiv V(\mathbf{r})$, and that the nonlinear ($|\psi|^2$) term is absent. Then our GPE reduces to the linear Schrodinger equation, that is,

$$i\frac{\partial\psi}{\partial t} = H\psi \tag{5}$$

where $H = -\frac{1}{2}\nabla^2 + V(\mathbf{r})$ is the corresponding Hamiltonian operator (introduced as a shorthand notation)[2]. We may integrate this

[2]Note that the chemical potential does not appear in the Hamiltonian; when the nonlinearity is zero is reduces to zero.

differential equation via separation of variables. Integrating from an initial wavefunction at time t, $\psi(\mathbf{r},t)$, to a later wavefunction at time $t = t+\Delta t$, $\psi(\mathbf{r},t+\Delta t)$, we obtain the explicit form of the time evolution[3],

$$\psi(\mathbf{r},t+\Delta t) = \exp(-i\Delta t H)\psi(\mathbf{r},t). \tag{6}$$

EXERCISE: Derive this form by integrating the differential equation (5) and hence convince yourself that this form only holds if H and V are time-independent.

We then make the following approximation, known as Cayley's form, for the time evolution operator,

$$\exp(-iH\Delta t) \approx \frac{1-\frac{i\Delta t}{2}H}{1+\frac{i\Delta t}{2}H}. \tag{7}$$

EXERCISE: Show that this relation holds up to and including first order in Δt. (Hint: you may assume that $\frac{i\Delta t}{2}H \ll 1$.)

Combining Equations (6) and (7) we can then write,

$$\left[1-\frac{i\Delta t}{2}H\right]\psi(\mathbf{r},t+\Delta t) = \left[1+\frac{i\Delta t}{2}H\right]\psi(\mathbf{r},t). \tag{8}$$

The physical interpretation of this is that the future wavefunction $\psi(\mathbf{r},t+\Delta t)$ is propagated *back* in time by half a time step, while the current wavefuntion $\psi(\mathbf{r},t)$ is propagated *forward* by half a time step. At this central time, both sides should be approximately equal.

3.2 Time-dependent Hamiltonian

The general GPE Hamiltonian in dimensionless form is,

$$H = -\frac{1}{2}\nabla^2 + V(\mathbf{r},t) + |\psi(\mathbf{r},t)|^2 - 1 \tag{9}$$

[3]This exact integration is only possible if $H \equiv H(\mathbf{r})$ and $V \equiv V(\mathbf{r})$, i.e. not functions of time. We will see later how we can approximate this when faced with the GPE Hamiltonian (which is time-dependent).

This is certainly time-dependent through the presence of the $|\psi(\mathbf{r},t)|^2$ term. The potential V may also be time-dependent, e.g. a moving obstacle. To account for the time-dependent Hamiltonian, we rewrite Equation (8) as,

$$\left[1-\frac{i\Delta t}{2}H(t+\Delta t)\right]\psi(\mathbf{r},t+\Delta t)=\left[1+\frac{i\Delta t}{2}H(t)\right]\psi(\mathbf{r},t), \quad (10)$$

i.e. we now include the future Hamiltonian $H(t+\Delta t)$ on the left side.

The aim is to solve this equation to obtain the future wavefunction $\psi(\mathbf{r},t+\Delta t)$. However, this requires knowledge of $H(\mathbf{r},t+\Delta t)$, which itself depends on the unknown $\psi(\mathbf{r},t+\Delta t)$! To overcome this "catch 22" problem, we calculate an intermediate wavefunction by setting $H(\mathbf{r},t+\Delta t)=H(\mathbf{r},\Delta t)$ in Equation (10). This intermediate wavefunction is then used to update the future Hamiltonian, and the next wavefunction solution is found. This intermediate process can be iterated until convergence of the new wavefunction. Two iterations of this intermediate process usually gives sufficient accuracy for this step of the algorithm.

3.3 Time discretization and time steps

In the above, we have considered a small interval of time Δt. We will consider the time variable in our simulation to be discretized into such regular intervals, i.e. time proceeds in the series $t=0,\Delta t,2\Delta t,3\Delta t$, etc. We denote the time index n such that $t=n\Delta t$. We also now introduce the shorthand notations for the Hamiltonian and wavefunction at the nth time step as H_n and ψ_n.

4 Crank-Nicolson Method: 1D System

For simplicity we first show how to spatially discretize and evolve the wavefunction in 1D. We will then extend this to 2D.

4.1 Discretizing along a line

Consider a 1D wavefunction $\psi(\mathbf{r}, t) \equiv \psi(x, t)$. We consider it to be defined over a linear region $[x_L, x_U]$ (L denoting the *lower* boundary and U denoting the *upper* boundary). We discretize the region into N grid points, with spacing Δx. We label the grid with index i (which runs from 1 to N) such that x_i denotes the position at the ith grid point,

$$x_i = x_L + (i-1)\Delta x. \tag{11}$$

At the ith grid point the wavefunction is $\psi(x_i)$, for which we introduce the shorthand notation ψ_i. Then the whole wavefunction (at a given time) is defined by the array $[\psi_1, \psi_2, \psi_3, ..., \psi_N]$. The discretization of $\psi(x)$ along the line is illustrated in Figure 1.

EXERCISE: Express Δx in terms of x_L, x_U and N.

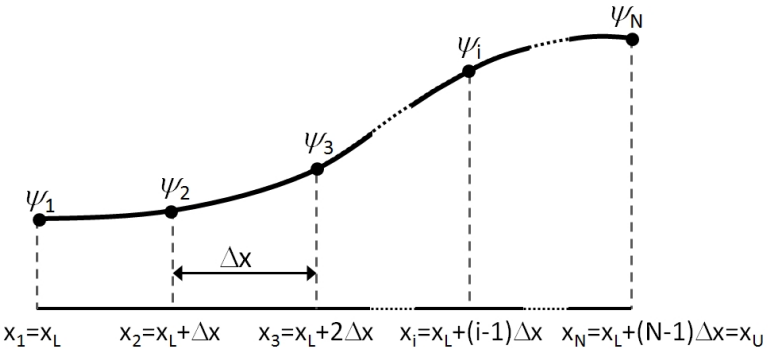

Figure 1: Discretization of $\psi(x)$ onto a linear grid.

4.2 Discrete form of the GPE Hamiltonian

The time evolution step for the GPE given in Equation (10) requires knowledge of the GPE Hamiltonian, which in 1D is given by,

$$H = -\frac{1}{2}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V(x,t) + |\psi(x,t)|^2 - 1. \tag{12}$$

On our discretized grid, this Hamiltonian must be evaluated at each point in the grid. For the moment, we will consider this to be done at a fixed time. Consider the ith point on the grid. The potential term here is $V_i = V(x_i)$ and the nonlinear term is $|\psi_i|^2 = |\psi(x_i)|^2$. The second derivative term requires more thought.

We approximate the second derivative term via finite-difference methods. First consider taking the single derivative at point i. We can approximate this via,

$$\frac{d\psi_i}{dx} \approx \delta_x \psi_i \equiv \frac{\psi_{i+\frac{1}{2}} - \psi_{i-\frac{1}{2}}}{\Delta x}, \tag{13}$$

where δ_x denotes the finite-differencing operator. This represents taking the gradient from a straight-line approximation between the wavefunction at positions a half-step to the left and a half-step right of the ith point.

Performing this finite-differencing operation as second time gives us an approximation for the second-derivative,

$$\frac{d^2\psi_i}{dx^2} \approx \delta_x^2 \psi_i \equiv \frac{\psi_{i+1} - 2\psi_i + \psi_{i-1}}{\Delta x^2}. \tag{14}$$

EXERCISE: Show that $\delta_x^2\psi_i$ does indeed lead to the expression on the far right of the above equation.

We can then write the Hamiltonian at point i as,

$$H_i = -\frac{1}{2}\delta_x^2 + V_i + |\psi_i|^2 - 1 \tag{15}$$

4.3 Crank-Nicolson result for a wavefunction point

We have now discretized the wavefunction in time and space, and have an approximate form for the Hamitonian. In other words, we have all the ingredients to numerically apply the time evolution equation (10). Applying this to the ith point in space and the nth step in time we have,

$$\left[1+\frac{i\Delta t}{2}\left(\frac{1}{2}\delta_x^2+U_i^{n+1}\right)\right]\psi_i^{n+1}=\left[1-\frac{i\Delta t}{2}\left(\frac{1}{2}\delta_x^2+U_i^{n}\right)\right]\psi_i^{n}. \tag{16}$$

where $U_i^n = 1-V_i^n-|\psi_i^n|^2$ is introduced for shorthand notation. This equation represents the Crank-Nicolson method. It is the crucial equation which enables us to evolve the GPE in time.

4.4 Crank-Nicolson result in matrix form

The time-evolution step above applies to all points in the grid, i.e. to the wavefunction array $[\psi_1, \psi_2, ...\psi_N]$. As such we can write it in matrix form.

First, though, let us extend the finite-differencing operation to apply to all points in the grid. We can write this full operation on ψ in matrix form as,

$$\delta_x^2\psi=\begin{pmatrix} -2 & 1 & 0 & 0 & \ddots \\ 1 & -2 & 1 & 0 & \ddots \\ 0 & 1 & -2 & 1 & \ddots \\ 0 & 0 & 1 & -2 & \ddots \\ \ddots & \ddots & \ddots & \ddots & \ddots \end{pmatrix}\begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \\ \vdots \end{pmatrix}.$$

We are now in a position to extend Equation (16) to matrix form. First, we introduce the shorthand notation $P^n = U^n - \frac{1}{\Delta x^2}$. Then

we can write,

$$\begin{pmatrix} 1+\frac{i\Delta t}{2}P^{n+1} & \frac{i\Delta t}{4\Delta x^2} & 0 & 0 & \ddots \\ \frac{i\Delta t}{4\Delta x^2} & 1+\frac{i\Delta t}{2}P^{n+1} & \frac{i\Delta t}{4\Delta x^2} & 0 & \ddots \\ 0 & \frac{i\Delta t}{4\Delta x^2} & 1+\frac{i\Delta t}{2}P^{n+1} & \frac{i\Delta t}{4\Delta x^2} & \ddots \\ \ddots & \ddots & \ddots & \ddots & \ddots \end{pmatrix} \begin{pmatrix} \psi_1^{n+1} \\ \psi_2^{n+1} \\ \psi_3^{n+1} \\ \vdots \end{pmatrix}$$

$$= \begin{pmatrix} 1-\frac{i\Delta t}{2}P^{n} & -\frac{i\Delta t}{4\Delta x^2} & 0 & 0 & \ddots \\ -\frac{i\Delta t}{4\Delta x^2} & 1-\frac{i\Delta t}{2}P^{n} & -\frac{i\Delta t}{4\Delta x^2} & 0 & \ddots \\ 0 & -\frac{i\Delta t}{4\Delta x^2} & 1-\frac{i\Delta t}{2}P^{n} & -\frac{i\Delta t}{4\Delta x^2} & \ddots \\ \ddots & \ddots & \ddots & \ddots & \ddots \end{pmatrix} \begin{pmatrix} \psi_1^{n} \\ \psi_2^{n} \\ \psi_3^{n} \\ \vdots \end{pmatrix}.$$

Or, multipying out the RHS,

$$\begin{pmatrix} 1+\frac{i\Delta t}{2}P^{n+1} & \frac{i\Delta t}{4\Delta x^2} & 0 & 0 & \ddots \\ \frac{i\Delta t}{4\Delta x^2} & 1+\frac{i\Delta t}{2}P^{n+1} & \frac{i\Delta t}{4\Delta x^2} & 0 & \ddots \\ 0 & \frac{i\Delta t}{4\Delta x^2} & 1+\frac{i\Delta t}{2}P^{n+1} & \frac{i\Delta t}{4\Delta x^2} & \ddots \\ \ddots & \ddots & \ddots & \ddots & \ddots \end{pmatrix} \begin{pmatrix} \psi_1^{n+1} \\ \psi_2^{n+1} \\ \psi_3^{n+1} \\ \vdots \end{pmatrix}$$

$$\begin{pmatrix} \left[1-\frac{i\Delta t}{2}\left(U^n-\frac{1}{\Delta x^2}\right)\right]\psi_1^n - \frac{i\Delta t}{4\Delta x^2}\psi_2^n \\ -\frac{i\Delta t}{4\Delta x^2}\psi_1^n + \left[1-\frac{i\Delta t}{2}\left(U^n-\frac{1}{\Delta x^2}\right)\right]\psi_2^n - \frac{i\Delta t}{4\Delta x^2}\psi_3^n \\ -\frac{i\Delta t}{4\Delta x^2}\psi_2^n + \left[1-\frac{i\Delta t}{2}\left(U^n-\frac{1}{\Delta x^2}\right)\right]\psi_3^n - \frac{i\Delta t}{4\Delta x^2}\psi_4^n \\ \vdots \end{pmatrix}.$$

The size of the matrix system is determined by the number of grid points N: the 2D matrix on the left is of size $N \times N$ and the two arrays are of length N. An important observation is that the 2D matrix is sparse, with most values in the matrix being zero. What's more, the 2D matrix is only non-zero along the diagonal (from top left to bottom right), and the two diagonal lines adjacent to this. We call such a matrix a *tridiagonal matrix*.

As such the matrix equation we have is of the more general form,

$$\mathbf{A_{td}X} = \mathbf{B},$$

where $\mathbf{A_{td}}$ denotes the tridiagonal matrix, $\mathbf{B}$ is a known array and $\mathbf{X}$ is the array to be found. This is a common matrix problem and it can be solved using a well-established tridiagonal matrix algorithm [2, 3]. By solving it, we obtain the matrix $\mathbf{X}$, i.e. the new wavefunction ψ^{n+1} at the future time.

5 Crank-Nicolson Method: 2D System

5.1 Discretizing on a 2D grid

We now consider the case for a two-dimensional wavefunction $\psi(x, y)$ existing in a box extending over the region $[x_L, x_U] \times [y_L, y_U]$. We discretized this region into a uniform lattice of grid points. There exist N_x points in the x-direction with spacing Δx, and N_y points in the y-direction with spacing Δy. i and j are now the indices for the x and y positions, where,

$$x_i = x_L + (i-1)\Delta x \quad \text{and} \quad y_j = y_L + (j-1)\Delta y \tag{17}$$

The wavefunction is defined at these grid points. At the (i, j) grid point, we denote the position as (x_i, y_j) and the wavefunction as $\psi_{i,j} \equiv \psi(x_i, y_j)$. We illustrate this spatial discretization in Figure 2.

5.2 Crank-Nicolson result for a wavefunction point

In 2D the GPE Hamiltonian features the Laplacian $\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}$. Under the finite-difference scheme we showed earlier that we can make the approximation $\frac{\partial^2}{\partial x^2} \approx \delta_x^2$. Similarly, in the y-direction was can make the corresponding approximation $\frac{\partial^2}{\partial y^2} \approx \delta_y^2$, where the operator δ_y has the analogous definition to δ_x. Then, on this 2D

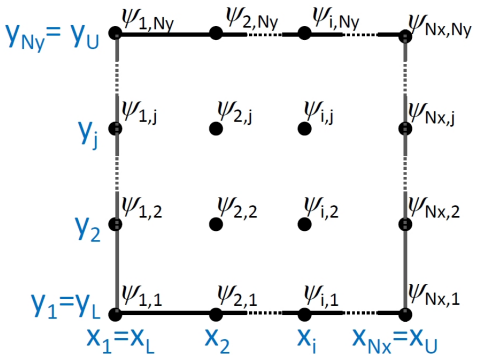

Figure 2: Discretization of $\psi(x, y)$ onto a 2D grid.

grid our finite-difference approximation of the derivatives are,

$$\delta_x \psi_{i,j} \equiv \frac{\psi_{i+\frac{1}{2},j} - \psi_{i-\frac{1}{2},j}}{\Delta x} \quad , \quad \delta_x^2 \psi_{i,j} \equiv \frac{\psi_{i+1,j} - 2\psi_{i,j} + \psi_{i-1,j}}{\Delta x^2}$$
$$\delta_y \psi_{i,j} \equiv \frac{\psi_{i,j+\frac{1}{2}} - \psi_{i,j-\frac{1}{2}}}{\Delta y} \quad , \quad \delta_y^2 \psi_{i,j} \equiv \frac{\psi_{i,j+1} - 2\psi_{i,j} + \psi_{i,j-1}}{\Delta y^2}.$$

In discretised form, Equation (8) becomes,

$$\left[1 + \frac{i\Delta t}{2}\left(\frac{\delta_x^2}{2} + \frac{\delta_y^2}{2} + U_{ij}\right)\right]\psi_{ij}^{n+1} = \left[1 - \frac{i\Delta t}{2}\left(\frac{\delta_x^2}{2} + \frac{\delta_y^2}{2} + U_{ij}\right)\right]\psi_{ij}^{n},$$

where $U_{ij}^n = 1 - V_{ij}^n - |\psi_{ij}^n|^2$. Each Hamiltonian operator (the bit in the square brackets) is now a function of x and y.

5.3 Alternating direction method

Since we are only working to an accuracy of Δt^2 (see Equation (7)) we can split the operators into the two separate directional compo-

nents, i.e.,

$$\left[1 \pm \frac{i\Delta t}{2}\left(\frac{\delta_x^2}{2} + \frac{\delta_y^2}{2} + U_{ij}\right)\right] \approx \left[1 \pm \frac{i\Delta t}{2}\left(\frac{\delta_x^2}{2} + \frac{U_{ij}}{2}\right)\right]\left[1 \pm \frac{i\Delta t}{2}\left(\frac{\delta_y^2}{2} + \frac{U_{ij}}{2}\right)\right]. \quad (18)$$

Then the two-dimensional problem is reduced to an array of one-dimensional equations. The method is to evolve the wavefunction in one dimension and then switch to the other. This is the *alternating direction method* approach.

5.4 A further approximation

We can make one final modification to the time evolution operator. Again within the limit of Δt^2 accuracy it is feasible to drop the potential/nonlinear terms in all but one of the directional operators, say the x-direction, to give

$$\left[1 + \frac{i\Delta t}{2}\left(\frac{\delta_x^2}{2} + \frac{\delta_y^2}{2} + U_{ij}\right)\right] \approx \left[1 + \frac{i\Delta t}{2}\left(\frac{\delta_x^2}{2} + U_{ij}\right)\right]\left[1 + \frac{i\Delta t}{4}\delta_y^2\right].$$

Recall from Section 3.2 that for a time-dependent Hamiltonian, we must perform an iterative intermediate step when evolving the wavefunction (so as to update the future Hamiltonian). With the above approximation, the Hamiltonian in the x-direction remains time-dependent but the Hamiltonian in the y-direction is time-independent. Thus we must perform this iterative intermediate step only when evolving the x-direction of the system.

6 Boundary Conditions

It is critical to set appropriate boundary conditions for a given simulation. To facilitate the setting of boundary conditions, the 2D grid

features a perimeter of extra points along $i = 0$, $i = N_x + 1$, $j = 0$ and $j = N_y + 1$. The wavefunction is defined at these points, but they are not updated in the time evolution operation (which only applies to the points over the range $[1, N_x] \times [1, N_y]$). Although they are not directly updated, they take part in the time evolution of the system since they are used to determine the spatial derivatives in the Hamiltonian. As such the presence of these points are "felt" across the rest of the system.

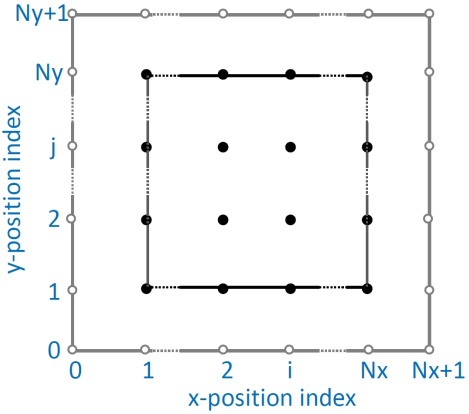

Figure 3: An outer set of grid points, the perimeter points (shown in grey), are introduced to facilitate setting the boundary conditions.

The simplest conditions are *fixed boundary conditions*. Since these perimeter points are not updated, if we initially set the wavefunction at these points to some value, they will remain fixed at that value throughout the subsequent evolution.

7 Stability and Convergence

It is dangerous to blindly assume that the results given by this method are correct. It is of crucial importance to ensure that numerical results obtained are stable and converged. Recall that the governing time-evolution equation that our numerical method is based on, Equation (8), is accurate to the order of $(\Delta t)^2$. Thus Δt is a particularly important factor in ensuring stability and accuracy of the method. A rule of thumb is that the algorithm is *stable* provided $\Delta t < \Delta x^2/2$ in 1D or $\Delta t < \Delta x \Delta y/2$ in 2D [2]. By *stable*, we mean that the simulation will be free from wacky behaviour where the wavefunction may suddenly "blow up".

The simulation may be stable but is not necessarily well-converged. Indeed the degree of convergence we require often depends on the level of detail we require. A good measure of stability and converge is the particle number. Some loss (or even gain!) of particles is inevitable in a numerical simulation, but this should typically be very very small, e.g. the quantity $\Delta N/N(t=0)$, where ΔN is the change in particle number during a simulation, should typically be of the order of 10^{-6} or less. Another measure is the system energy. This should, in principle, remain constant if the potential is time-independent. The numerical evaluation of the particle number and system energy is detailed in the following section.

Typical time and space steps which could be used are $\Delta t = 0.02$ and $\Delta x = 0.2$. However, it is critical to verify that any set of simulations are well-converged. An example strategy is to run a trial simulation with greater time and space resolution (e.g. half the grid spacing and quarter the time step) and ensure that the results are not markedly different.

8 Evaluating Particle Number & Energy

Particle number

The number of particles described by the wavefunction is given by

the integral,

$$N = \int |\psi|^2 \, \mathrm{d}x \, \mathrm{d}y. \tag{19}$$

During real time propagation of the GPE, the total number of particles (in dimensionless units) must be conserved. This is true under *exact* integration but of course we make various approximations to solve the GPE and as such the particle number can be expected to deviate slightly over time. In our numerical system, we may employ the trapezium rule to approximate this integral as,

$$N \approx \Delta x \Delta y \sum_{i,j} |\psi_{i,j}|^2. \tag{20}$$

Total energy

The total energy of the system is given by the integral,

$$E = \int \left(\frac{1}{2} |\nabla \psi|^2 + V|\psi|^2 + \frac{1}{2}|\psi|^4 \right) \, \mathrm{d}x \, \mathrm{d}y. \tag{21}$$

To determine the $|\nabla\psi|^2$-term numerically, it is convenient to express ψ in terms of its real and imaginary components as $\psi = \psi^R + i\psi^I$. This leads to,

$$|\nabla\psi|^2 = (\nabla\psi^R)^2 + (\nabla\psi^I)^2.$$

And using $\nabla = \mathbf{i}\frac{\partial}{\partial x} + \mathbf{j}\frac{\partial}{\partial y}$ we can obtain,

$$|\nabla\psi|^2 = \left(\frac{\partial\psi^R}{\partial x}\right)^2 + \left(\frac{\partial\psi^R}{\partial y}\right)^2 + \left(\frac{\partial\psi^I}{\partial x}\right)^2 + \left(\frac{\partial\psi^I}{\partial y}\right)^2$$

We can then approximate each single derivative using the finite different approach, e.g,

$$\frac{\partial\psi^R_{i,j}}{\partial x} \approx \frac{\psi^R_{i+1,j} - \psi^R_{i-1,j}}{2\Delta x} \quad \text{and} \quad \frac{\partial\psi^R_{i,j}}{\partial y} \approx \frac{\psi^R_{i,j+1} - \psi^R_{i,j-1}}{2\Delta y},$$

and similarly for the derivatives of ψ^I.

Numerically, we may then approximate the energy integral with the discrete form,

$$E \approx \Delta x \Delta y \sum_{i,j} \left\{ \frac{1}{2} \left(\frac{\psi^R_{i+1,j} - \psi^R_{i-1,j}}{2\Delta x} \right)^2 + \frac{1}{2} \left(\frac{\psi^R_{i,j+1} - \psi^R_{i,j-1}}{2\Delta y} \right)^2 \right.$$
$$\left. + \frac{1}{2} \left(\frac{\psi^I_{i+1,j} - \psi^I_{i-1,j}}{2\Delta x} \right)^2 + \frac{1}{2} \left(\frac{\psi^I_{i,j+1} - \psi^I_{i,j-1}}{2\Delta y} \right)^2 + V_{i,j} |\psi_{i,j}|^2 + \frac{1}{2} |\psi_{i,j}|^4 \right\} .$$

9 Obtaining Static Solutions

In certain limited cases, the static solution of the system may be found analytically. For example, in the absence of trapping potential the static solution of the GPE is $\psi = 1$. However, in general, the static solution must be found by solving the GPE numerically.

9.1 Imaginary time propagation of the GPE

A reliable and easily-implemented method of obtaining the ground state of the system is by propagation in imaginary time. Making the substitution $\Delta t \to -i\Delta t$ in the GPE, the time evolution equation (6) becomes,

$$\psi(\mathbf{r}, t + \Delta t) = e^{-H\Delta t} \psi(\mathbf{r}, t). \tag{22}$$

Since H and Δt are positive, this implies that the wavefunction decays over time.

We can express $\psi(t)$ as a superposition of eigenstates $\phi_m(\mathbf{r})$ of the system, with time-dependent amplitudes $a_m(t)$ and eigenenergies $E_m(t)$, i.e.

$$\psi(\mathbf{r}, t) = \sum_m a_m(t) \phi_m(\mathbf{r}). \tag{23}$$

Using the relation $H\phi_m = (E_m - \mu)\phi_m$, we obtain,

$$\psi(\mathbf{r}, t + \Delta t) = \sum_m a_m(t)\phi_m(\mathbf{r}) \exp[-(E_m - \mu]\Delta t). \quad (24)$$

The term $\exp[-(E_m - \mu)\Delta t]$ causes the eigenstates with $E_m \geq \mu$ to decay over time and only the eigenstate with $E_m = \mu$ remains. In other words, if we begin from some trial solution and evolve this in imaginary time, then the system will converge to the ground state of the system (with chemical potential μ).

9.2 Generating a vortex state in imaginary time

A vortex state in a 2D system, with rotational charge q, is generated by propagating the GPE in imaginary time, subject to a $2\pi q$ azimuthal phase slip. For example, to create a singly-charged vortex at the origin, the wavefunction should be modified at each time step via,

$$\psi \rightarrow |\psi| \exp[i \tan^{-1}(y/x)]. \quad (25)$$

To create a vortex line in 3D, the phase must be enforced along the desired axis. If the resulting vortex state is time-dependent, then, when run in real time, a small amount of transient sound will be released as the vortex initially accelerates to its moving state.

References

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