Appendix A
Simulating the 1D GPE

The GPE is a nonlinear partial differential equation, and its solution must, in general, be obtained numerically. A variety of numerical methods exist to solve the GPE, including those based on Runge–Kutta methods, the Crank–Nicolson method and the split-step Fourier method.[1] The latter (also known as the time-splitting spectral method) is particularly compact and efficient, and here we apply it to the 1D GPE. Furthermore, we introduce the imaginary time method for obtaining ground state solutions. Basic Matlab code is provided.

A.1 Split-Step Fourier Method

The split-step fourier method is well-established for numerically solving the time-dependent Schrodinger equation, written here in one-dimension,

$$i\hbar\frac{\partial\psi(x,t)}{\partial t} = \hat{H}\psi(x,t). \tag{A.1}$$

The Hamiltonian $\hat{H}$ can be expressed as $\hat{H} = \hat{T} + \hat{V}$, where $\hat{T} \equiv -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$ and $\hat{V} \equiv V(x)$ are the kinetic and potential energy operators. Integrating from t to $t + \Delta t$ (and noting the time-independence of the Hamiltonian) leads to the time-evolution equation,

$$\psi(x, t + \Delta t) = e^{-i\Delta t\hat{H}/\hbar}\psi(x,t). \tag{A.2}$$

The operators T and V do not commute, hence $e^{-i\Delta t\hat{H}/\hbar} \neq e^{-i\Delta t\hat{T}/\hbar}e^{-i\Delta t\hat{V}/\hbar}$. Nonetheless, the following approximation,

$$e^{-i\Delta t\hat{H}/\hbar}\psi \approx e^{-i\Delta t\hat{V}/2\hbar}e^{-i\Delta t\hat{T}/\hbar}e^{-i\Delta t\hat{V}/2\hbar}\psi, \tag{A.3}$$

[1] A. Minguzzi, S. Succi, F. Toschi, M.P. Tosi, P. Vignolo, Phys. Rep. **395**, 223 (2004).

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holds with error $\mathcal{O}(\Delta t^3)$. In position space $\hat{V}$ is diagonal, and so the operation $e^{-i\Delta t\hat{V}/2\hbar}\psi$ simply corresponds to multiplication of $\psi(x,t)$ by $e^{-i\Delta t V(x)/2\hbar}$. Although $\hat{T}$ is not diagonal in position space, it becomes diagonal in reciprocal space. Conversion to reciprocal space is achieved by taking the Fourier transform $\mathcal{F}$ of the wavefunction $\tilde{\psi}(k,t) = \mathcal{F}[\psi(x,t)]$, where k denotes the 1D wavevector. Then the kinetic energy operation corresponds to multiplication of $\tilde{\psi}(k,t)$ by $e^{-i\hbar\Delta t k^2/2m}$. Thus Eq. (A.3) can be written as,

$$\psi(x,t+\Delta t) \approx e^{-\frac{i}{2\hbar}V(x)\Delta t}\cdot\mathcal{F}^{-1}\left[e^{-\frac{i\hbar k^2}{2m}\Delta t}\cdot\mathcal{F}\left[e^{-\frac{i}{2\hbar}V(x)\Delta t}\cdot\psi(x,t)\right]\right]. \qquad \text{(A.4)}$$

In practice, the computational expense of performing forward and backward Fourier transforms to evaluate Eq. (A.3) is small (particularly when using numerical fast Fourier transform techniques) compared to the significant expense of evaluating the kinetic energy term directly in position space. Note that the split-step method naturally incorporates periodic boundary conditions.

The above method was developed for the linear Schrodinger equation with time-independent Hamiltonian. Remarkably, it holds for the GPE (despite its nonlinearity and time-dependent Hamiltonian) under the replacement $V(x) \mapsto V(x) + g|\psi|^2$. Errors of $\mathcal{O}(\Delta t^3)$ are maintained, providing the most up-to-date ψ is always employed during the sequential operations in Eq. (A.4).[2]

A.2 1D GPE Solver

We now outline the approach to solve the 1D GPE using the split-step method, with reference to the Matlab code included below. To make the numbers more convenient, the GPE is divided through by $\hbar$ (equivalent to considering energy in units of $\hbar$). We consider a 1D box, discretized into grid points with spacing Δx (`dx`), and extending over the spatial range $x = [-M\Delta x, M\Delta x]$, where M (`M`) is a positive integer. Position is described by a vector x_i (`x`), defined as $x_i = -M\Delta x + (i-1)\Delta x$, with $i = 1,\ldots,2M+1$. The potential $V(x)$ is defined as the vector $V_i = V(x_i)$. Starting from the initial time, the wavefunction $\psi(x)$, represented by the vector $\psi_i = \psi(x_i)$ (`psi`), is evolved over the time interval Δt (`dt`) by evaluating Eq. (A.4) numerically by replacing the Fourier transform $\mathcal{F}$ (and its inverse $\mathcal{F}^{-1}$) by the discrete fast Fourier transform. Here, wavenumber is discretized into a vector k_i (`k`), defined as $k_i = -M\Delta k + (i-1)\Delta k$, with $\Delta k = \pi/M\Delta x$ (`dk`). This time iteration step is repeated N_t (`Nt`) times to find the solution at the desired final time.

The Matlab code below simulates a BEC of 5000 ^{87}Rb atoms with $a_s = 5.8\,\text{nm}$ and trapping frequencies $\omega_\perp = 2\pi\times 100\,\text{Hz}$ and $\omega_x = 2\pi\times 40\,\text{Hz}$. Starting from the narrow non-interacting ground state (Gaussian) profile, the condensate undergoes oscillating expansions and contractions, due to the competition between repulsive

[2] J. Javanainen, J. Ruostekoski, J. Phys. A **39**, L179 (2006).

interactions and confining potential. Note—under different scenarios, reduced time and grid spacings may be required to ensure numerical convergence.

```
% SOLVES THE 1D GPE VIA THE SPLIT-STEP FOURIER METHOD
clear all;clf; %Clear workspace and figure

hbar=1.054e-34;amu=1.660538921e-27; %Physical constants
m=87*amu;as=5.8e-9; %Atomic mass; scattering length
N=1000;wr=100*2*pi;wx=40*2*pi; %Atom number; trap frequencies

M=200; Nx=2*M+1;
dx=double(2e-7); x=(-M:1:M)*dx; %Define spatial grid
dk=pi/(M*dx); k=(-M:1:M)*dk; %Define k-space grid
dt=double(10e-8); Nt=200000; %Define time step and number

lr=sqrt(hbar/(m*wr)); lx=sqrt(hbar/(m*wx)); %HO lengths
g1d=2*hbar*hbar*as/(m*lr^2); %1D interaction coefficient

V=0.5*m*wx^2*x.^2/hbar; %Define potential
psi_0=sqrt(N/lx)*(1/pi)^(1/4)*exp(-x.^2/(2*lx^2)); %Initial wavefunction

%[psi_0,mu] = get_ground_state(psi_0,dt,g1d,x,k,m,V); %Imaginary time

Nframe=100; %Data saved every Nframe steps
t=0; i=1; psi=psi_0; spacetime=[]; %Initialization

for itime=1:Nt %Time-stepping with split-step Fourier method
     psi=psi.*exp(-0.5*1i*dt*(V+(g1d/hbar)*abs(psi).^2));
     psi_k=fftshift(fft(psi)/Nx);
     psi_k=psi_k.*exp(-0.5*dt*1i*(hbar/m)*k.^2);
     psi=ifft(ifftshift(psi_k))*Nx;
     psi=psi.*exp(-0.5*1i*dt*(V+(g1d/hbar)*abs(psi).^2));
     if mod(itime,Nt/Nframe) == 0  %Save wavefunction every Nframe steps
       spacetime=vertcat(spacetime,abs(psi.^2)); t
     end
     t=t+dt;
end

subplot(1,3,1); %Plot potential
plot(x,V,'k'); xlabel('x (m)'); ylabel('V (J/hbar)');

subplot(1,3,2); %Plot initial and final density
plot(x,abs(psi_0).^2,'k',x,abs(psi).^2,'b');
legend('\psi(x,0)','\psi(x,T)');xlabel('x (m)');ylabel('|\psi|^2 (m^{-1})');

subplot(1,3,3); % Plot spacetime evolution as pcolor plot
dt_large=dt*double(Nt/Nframe);
pcolor(x,dt_large*(1:1:Nframe),spacetime); shading interp;
xlabel('x (m)'); ylabel('t (s)');
```

A.3 Imaginary Time Method

A convenient numerical method for obtaining ground state solutions of the Schrodinger equation/GPE is through imaginary time propagation. The wavefunction $\psi(x, t)$ can be expressed as a superposition of eigenstates $\phi_m(x)$ with time-dependent amplitudes $a_m(t)$ and energies $E_m(t)$, i.e. $\psi(x, t) = \sum_m a_m(t)\phi_m(x)$, for which, after the substitution $t \to -i\Delta t$, the evolution Eq. (A.3) becomes,

$$\psi(t + \Delta t) = e^{-\Delta t\hat{H}/\hbar}\psi(x, t) = \sum_m a_m(t)\phi_m(x)e^{-\Delta t E_m/\hbar}. \tag{A.5}$$

The amplitude of each eigenstate contribution decays over time, with the ground state (with lowest E_m) decaying the slowest. Thus, by renormalizing ψ after each iteration (to ensure the conservation of the desired norm/number of particles), ψ will evolve towards the ground state.

Convergence may be assessed by monitoring the chemical potential. This is conveniently evaluated using the relation $\mu = (\hbar/\Delta t) \ln |\psi(x, t)/\psi(x, t + \Delta t)|$ at some coordinate within the condensate; this relation is obtained by introducing the eigenvalue μ and imaginary time into Eq. (A.3).

The Matlab function `get_ground_state` below obtains the GPE ground state via imaginary time propagation. Uncommenting line 19 in the above GPE solver calls this function prior to real time propagation; as one expects, the profile remains static in time.

```
% SOLVES THE 1D GPE IN IMAGINARY TIME USING THE SPLIT-STEP METHOD
function [psi,mu] = get_ground_state(psi,dt,g1d,x,k,m,V)

hbar=1.054e-34; dx=x(2)-x(1); dk=2*pi/(x(end)-x(1));
N=dx*norm(psi).^2; Nx=length(x); psi_mid_old=psi((Nx-1)/2);
mu_old=1; j=1; mu_error=1;
 while mu_error > 1e-8
     psi=psi.*exp(-0.5*dt*(V+(g1d/hbar)*abs(psi).^2));
     psi_k=fftshift(fft(psi))/Nx;
     psi_k=psi_k.*exp(-0.5*dt*(hbar/m)*k.^2);
     psi=ifft(ifftshift(psi_k))*Nx;
     psi=psi.*exp(-0.5*dt*(V+(g1d/hbar)*abs(psi).^2));

     psi_mid=psi((Nx-1)/2);
     mu=log(psi_mid_old/psi_mid)/dt; mu_error=abs(mu-mu_old)/mu;

     psi=psi*sqrt(N)/sqrt((dx*norm(psi).^2));
    if mod(j,5000) == 0
        mu_error
     end
     if j > 1e8
         'no solution found'
         break
     end
     psi_mid_old=psi((Nx-1)/2); mu_old=mu; j=j+1;
 end
end
```

Problems

A.1 Obtain the ground-state density profiles for a 1D condensate under harmonic confinement with (i) no interactions, (ii) repulsive interactions and (iii) attractive interactions. Compare (ii) with the corresponding Thomas–Fermi profile.

A.2 Starting from the Gaussian harmonic oscillator ground state, release the non-interacting condensate into an infinite square well (achieve by setting the potential to a high value towards the edge of the box, and zero elsewhere). Repeat for repulsive and attractive interactions. How does the initial expansion (before reflection from the box walls) depend on the interactions?

Now simulate the longer-term behaviour. The wavefunction undergoes revivals, known as the Talbot effect, and forms a "quantum carpet".[3]

A.3 Form the ground state solution for a repulsively-interacting condensate in a harmonic trap. Excite a centre-of-mass ("sloshing") oscillation by shifting the trap by some distance at $t = 0$. Similarly, excite a monopole mode by slightly weakening the trap at $t = 0$. Extract the frequencies of these modes. Do the frequencies depend on the number of particles and the interaction sign/strength?

[3] I. Marzoli et al. Acta Phys. Slov. **48**, 323 (1998) [arXiv:quant-ph/9806033].

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