EDT Part Draft

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1 Exponential Time Differencing Scheme

In this chapter, the main time stepping method is introduced and applied to solve the equation over time. In this study, a method named Exponential Time Differencing Scheme and developed by Matthews and Cox is applied. Exponential Time Differencing Scheme is applied to solve an ODE involving both linear and non-linear terms, which can be generalized as:

$$\frac{du(t)}{dt} = Lu(t) + N(u(t), t) \tag{1.1}$$

where L is a linear operator acting on $u(t)$ and $N(u(t), t)$ is the non-linear term. To solve the ODE in (1.1), we first state an integrating factor $\mu = \exp(-Lt)$ and multiply both sides of (1.1) by μ to get a new equation

$$\frac{d}{dt}(\exp(-Lt)u(t)) = \exp(-Lt)N(u(t), t) \tag{1.2}$$

Suppose at the current time step $t\prime$, the non-linear term $N(u(t\prime), t\prime)$ is known as a constant and if we integrate both sides over $(t\prime, t\prime + \Delta t)$, the equation (1.2) becomes:

$$\exp(-Lt)u(t)\Big|_{t\prime}^{t\prime+\Delta t} = N(u(t\prime), t\prime)\int_{t\prime}^{t\prime+\Delta t} \exp(-Lt)dt \tag{1.3}$$

Finally, the density at the new time step $u(t\prime + \Delta t)$ can be calculated as

$$u(t\prime + \Delta t) = \exp(L\Delta t)u(t\prime) + (\exp(L\Delta t) - 1)N(u(t\prime), t\prime) \tag{1.4}$$

1.1 Calculating the Transportation Term

This section will mainly be focusing on simulating the transportation term using Exponential Time Differencing (ETD) scheme. For the interaction terms all equal to zero, the equation can be simplified as

$$u_t + \gamma \mathbf{e}_\phi \cdot \nabla_{\boldsymbol{x}} u = 0 \tag{1.5}$$

To simulate the gradient of u over the space, we can apply semidescrete Fourier transform with an assumption that the function u is bounded over $[-\pi, \pi]$ with periodic boundary condition, then

$$\hat{u}_{k_1,k_2}(\phi, t) = \alpha \int_{x_2=-\pi}^{\pi} \int_{x_1=-\pi}^{\pi} u\left(x_1, x_2, \phi, t\right) \exp\left(-i\left[k_1 x_1 + k_2 x_2\right]\right) \mathrm{d}x_1 \ \mathrm{d}x_2 \tag{1.6}$$

where k_1, k_2 are the wave number corresponding to x_1, x_2. The inverse Fourier transform is

$$u\left(x_1, x_2, \phi, t\right) = \beta \sum_{k_1=-\frac{N}{2}}^{\frac{N}{2}} \sum_{k_2=-\frac{N}{2}}^{\frac{N}{2}} \hat{u}_{k_1,k_2}(\phi, t) \exp\Big(i\left[k_1 x_1 + k_2 x_2\right]\Big) \tag{1.7}$$

where N is the discrete grid number and α, β are the normalization term during the transformation. To solve the function numerically, we are going to apply spectral method where we can apply Fast Fourier Transform and Inverse Fast Fourier Transform over a space grid with grid number N. Then we can get a coefficient matrix which does not change over time. The calculation of the coefficient matrix M will be explained in the following paragraphs.

If Fourier transform over the space is applied to (1.5), then $\nabla_x \hat{u} = (ik_1\hat{u}, ik_2\hat{u})$. Therefore, the equation becomes

$$\frac{\partial \hat{u}_{k_1,k_2}(\phi, t)}{\partial t} + i\gamma\Big[k_1\cos(\phi) + k_2\sin(\phi)\Big]\hat{u}_{k_1,k_2}(\phi, t) = 0 \tag{1.8}$$

Suppose that k_1, k_2 be known constants, and discretize ϕ over a grid between $[-\pi, \pi]$ with an even number m points such that $\phi_j = \frac{2\pi}{m} j$ with $j = -\frac{m}{2} \cdots \frac{m}{2} - 1$, the linear operator at the angle ϕ_j would be $L = -i\gamma[k_1 cos(\phi_j) + k_2 sin(\phi_j)]$. If we define $\hat{u}_{k_1,k_2,j} \equiv \hat{u}_{k_1,k_2}\left(\phi_j, t\right)$, (1.8) can be written as and ODE

$$\frac{\mathrm{d}\hat{u}_{k_1,k_2,j_1}(t)}{\mathrm{d}t} = \sum_{j_2=-\frac{m}{2}}^{\frac{m}{2}-1} M_{p_1,p_2}\hat{u}_{k_1,k_2,j_2} \tag{1.9}$$

where $j_1, j_2 \in (-\frac{m}{2}, \frac{m}{2})$ and $p_1 = j_1 + \frac{m}{2}$, $p_2 = j_2 + \frac{m}{2}$. Then M is a diagonal matrix having entries $M_{p_1,p_2} = L(k_1, k_2, \phi_{j_1})\delta_{j_1,j_2}$ with δ_{j_1,j_2} be the Dirac delta function. Then if we omit the known constants k_1, k_2, the system would become

$$\frac{d}{dt}\begin{bmatrix} \hat{u}_{-\frac{m}{2}} \\ \hat{u}_{-\frac{m}{2}+1} \\ \vdots \\ \hat{u}_{\frac{m}{2}-1} \end{bmatrix} = \begin{bmatrix} L(\phi_{-\frac{m}{2}}) & 0 & \cdots & 0 \\ 0 & L(\phi_{-\frac{m}{2}+1}) & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & L(\phi_{\frac{m}{2}-1}) \end{bmatrix} \begin{bmatrix} \hat{u}_{-\frac{m}{2}} \\ \hat{u}_{-\frac{m}{2}+1} \\ \vdots \\ \hat{u}_{\frac{m}{2}-1} \end{bmatrix} \tag{1.10}$$

where

$$M = \begin{bmatrix} L\left(\phi_{-\frac{m}{2}}\right) & 0 & \cdots & 0 \\ 0 & L\left(\phi_{-\frac{m}{2}+1}\right) & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & L\left(\phi_{\frac{m}{2}-1}\right) \end{bmatrix} \tag{1.11}$$

To solve the system (1.10), we can apply the ETD scheme, where we set the integrating factor $\mu = \exp(-Mt)$, the system cam be simplified as

$$\frac{\mathrm{d}}{\mathrm{d}t}(\exp(-Mt)\hat{u}) = 0 \tag{1.12}$$

If we integrate both sides over the current time step $t\prime$ and the new time step $t\prime + \Delta t$ to get

$$\exp(-M(t\prime + \Delta t))\hat{u}(t\prime + \Delta t) - \exp(-M(t\prime))\hat{u}(t\prime) = 0 \tag{1.13}$$

the right hand side remains zero since the non-linear term equals to zero. Then to solve for $u(t\prime + \Delta t)$ the equation becomes

$$\hat{u}(t\prime + \Delta t) = \exp(M\Delta t)\hat{u}(t\prime) \tag{1.14}$$

Finally, the inverse Fourier transform (stated in (1.7)) is applied to (1.14) to find the density function $u(t\prime + \Delta t)$ in real space.

1.2 Simulation of the Transportation Term

In this section, we are going to apply the EDT scheme to an initial condition of u

$$u_0(x_1, x_2, \phi) = \exp(\pi(\cos(x_1) + \cos(x_2))) \tag{1.15}$$

which is shown in Figure 1.

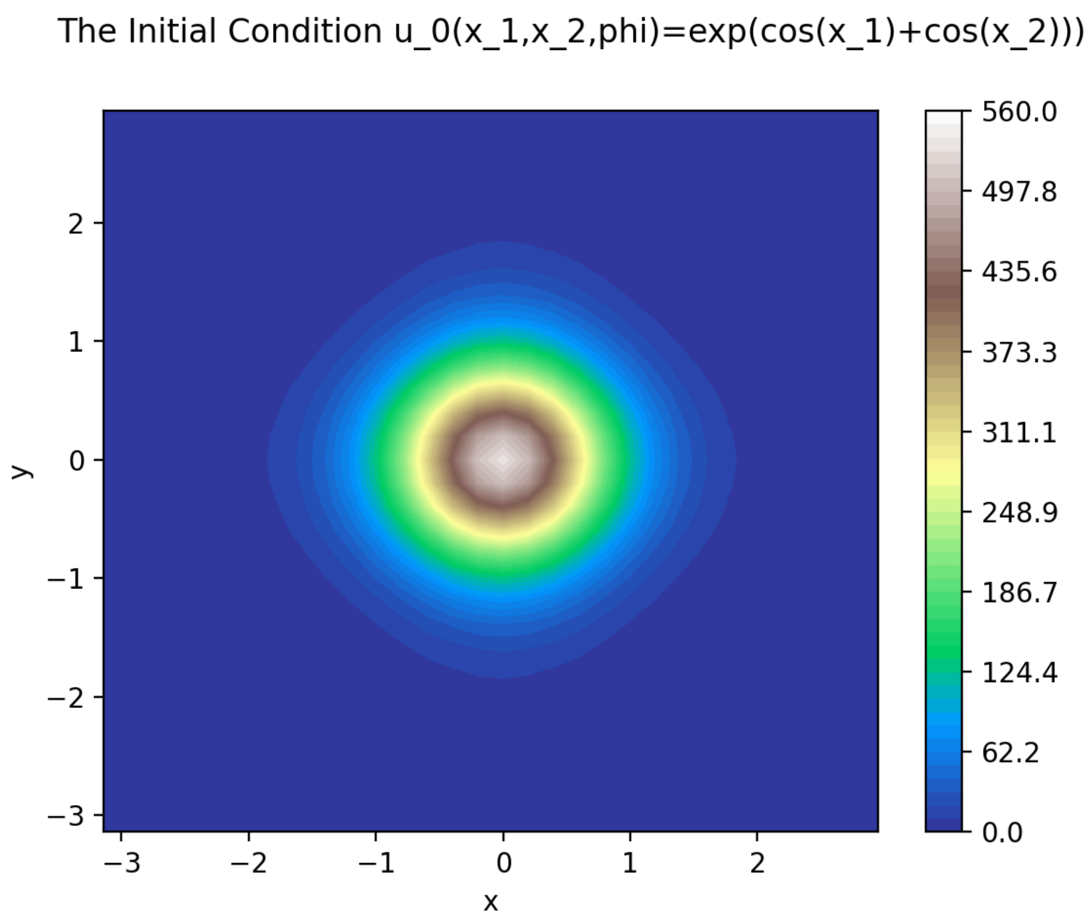
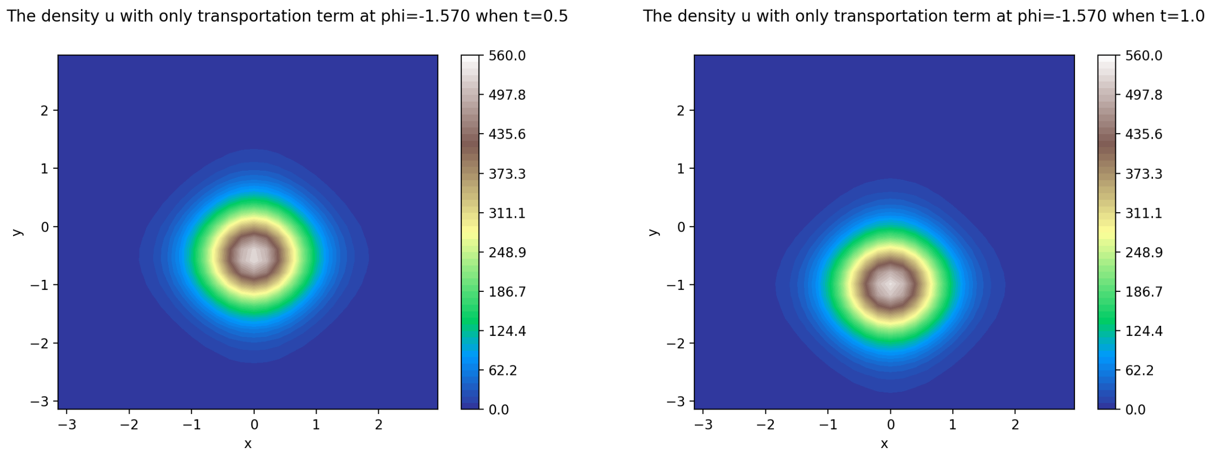
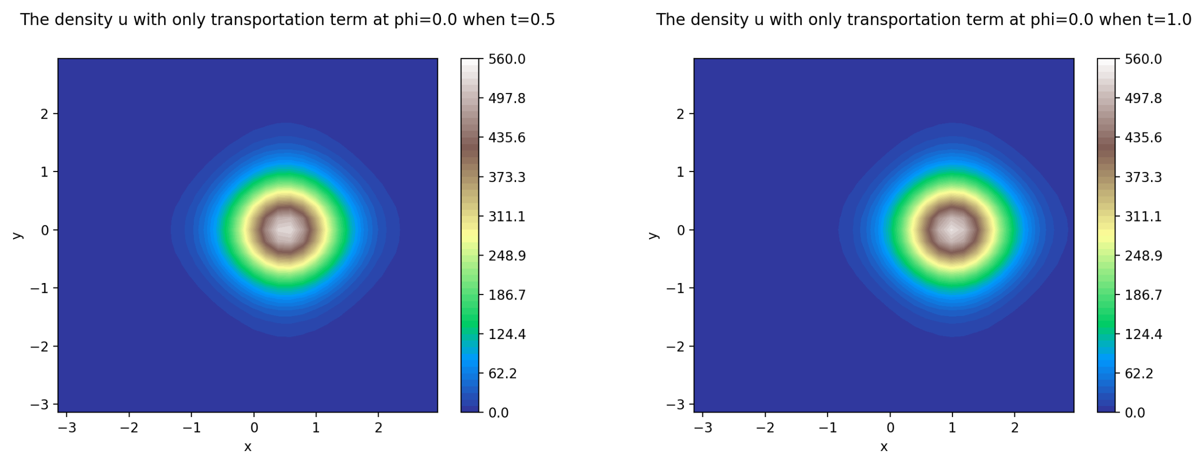


Figure 1: The Initial Condition $u_0(x_1, x_2, \phi) = \exp(\pi(\cos(x_1) + \cos(x_2)))$

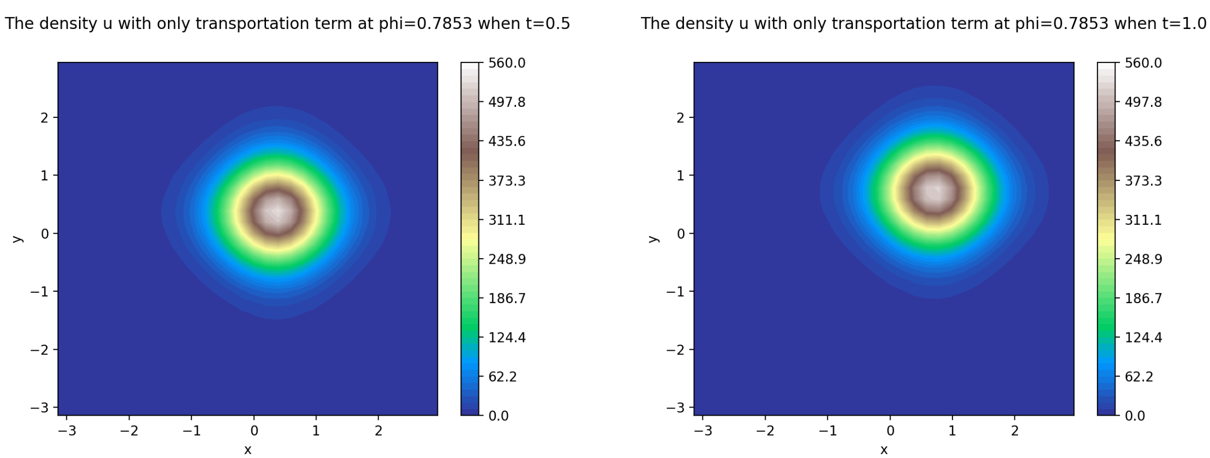
The initial condition u_0 stays the same for different ϕ. But as the time variable t gets larger, since the population is moving toward different directions, the density plot is also different at different ϕ (Figure 2).



(a) The Population Density Plot of $u(x_1, x_2, \phi = -\frac{\pi}{2})$ at $t = 0.5, 1$



(b) The Population Density Plot of $u(x_1, x_2, \phi = 0)$ at $t = 0.5, 1$



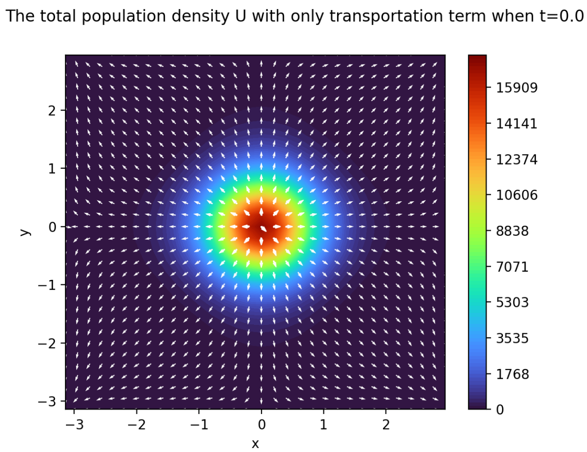
(c) The Population Density Plot of $u(x_1, x_2, \phi = \frac{\pi}{4})$ at $t = 0.5, 1$

Figure 2: The Population Density Plot of $u(x_1, x_2, \phi)$ with different ϕ at different t

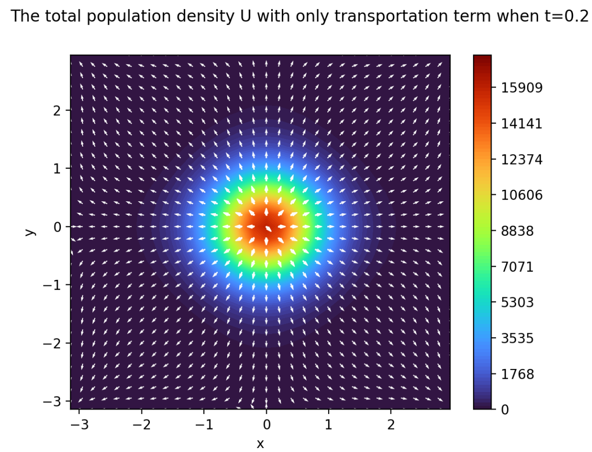
We can also look at the whole population density plot over different angles, where define the whole population $U(x_1, x_2, t)$ as

$$U(x_1, x_2, t) = \int_{-\pi}^{\pi} u(x_1, x_2, \phi, t) d\phi \tag{1.16}$$

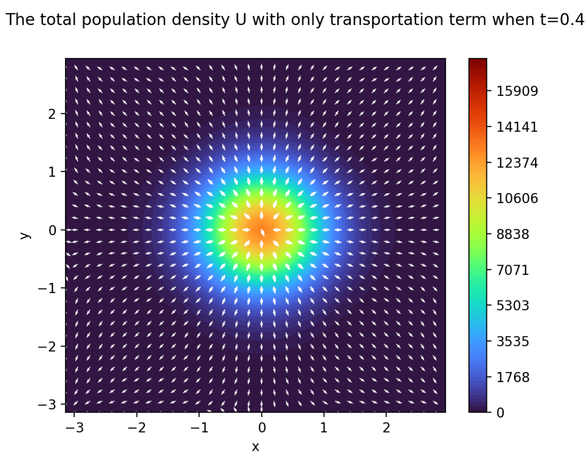
Also, let the arrows at the position x_1, x_2 represent the angle ϕ_{max} with the largest population. The thickness of the arrows varies with different density, where the thicker arrows represent a greater magnitude of density at $u(x_1, x_2, \phi_{max}, t)$. The plot is shown in Figure 3. In Figure 3, the initial population is concentrated in the center. Then the population starts to spread out from the center toward different directions.



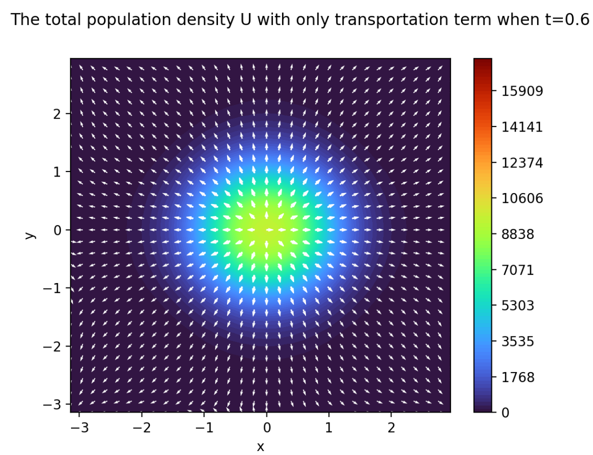
(a) when $t = 0$



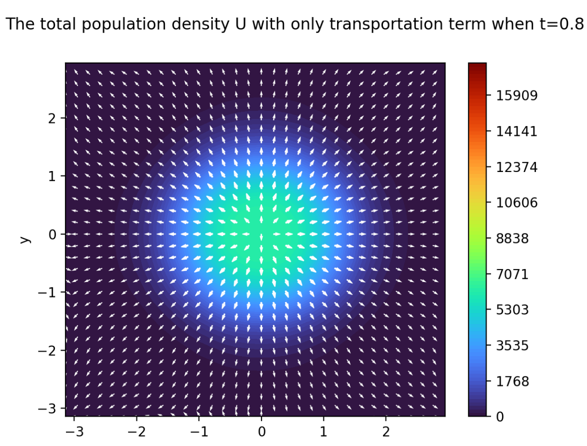
(b) when $t = 0.2$



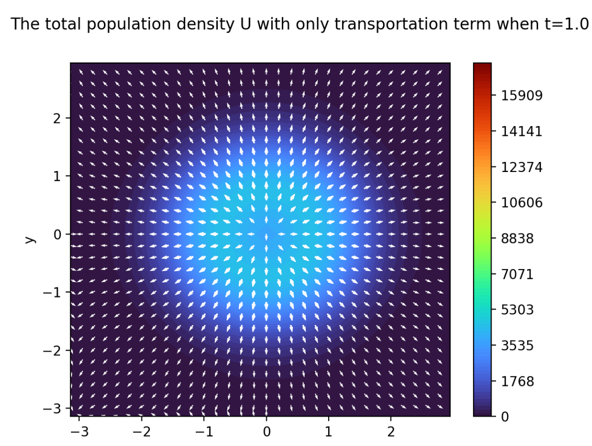
(c) when $t = 0.4$



(d) when $t = 0.6$



(e) when $t = 0.8$



(f) when $t = 1.0$

Figure 3: the Total Population Density U at different time t

1.3 Calculating the Interaction Term

As indicated in the last section, the interaction term is

$$N(u(t),t) = -\lambda(\phi, x_1, x_2)u\left(\phi, x_1, x_2, t\right) + \int_{\phi'=-\pi}^{\pi} S\Big(T\left(\phi, \phi', x_1, x_2\right)\Big)\, u\left(\phi', x_1, x_2, t\right) \mathrm{d}\phi' \tag{1.17}$$

with

$$\begin{aligned} T_j\left(\phi, \phi', X\right) &= q_j \int_{\mathbb{R}^2} K_j^d(X-S)K_j^o(\phi, X-S)w_j(\phi, \phi', X-S)U(S,t)\mathrm{d}S \\ \lambda_j(\phi, X) &= \int_{-\pi}^{\pi} T_j\left(\phi, \phi', X\right)\mathrm{d}\phi \end{aligned} \tag{1.18}$$

To compute the Turning function, we need to use the Convolution Theorem. First, we combine the Kernels $K_d(X-S), K_o(X-S,\phi)$ and the probability function $w_j(\phi, \phi', X-S)$ to form a new term $Kw_j(\phi, \phi', X-S)$ which does not change over time. The turning function is a convolution over space

$$T_j\left(\phi, \phi', X\right) = q_j \int_{\mathbb{R}^2} Kw_j(\phi, \phi', X-S)U(S,t)\mathrm{d}S \tag{1.19}$$

Then, we can apply the Fourier transform over the space term $X = (x_1, x_2)$.

$$\hat{T}_j\left(\phi, \phi', k_1, k_2\right) = \int_{\mathbb{R}^2} T_j\left(\phi, \phi', x_1, x_2\right)\exp(-ix_1k_1 - ix_2k_2)\mathrm{d}x_1\mathrm{d}x_2 \tag{1.20}$$

where k_1, k_2 are the wave numbers. Let $p_1 = x_1 - s_1, p_2 = x_2 - s_2, q_1 = s_1, q_2 = s_2$, then $x_1 = p_1 + q_1, x_2 = p_2 + q_2$

$$\begin{aligned} &\hat{T}_j\left(\phi, \phi', k_1, k_2\right) = q_j \int_{\mathbb{R}^2}\int_{\mathbb{R}^2} Kw_j(\phi, \phi', p_1, p_2)U(q_1, q_2, t)\mathrm{d}q_1\mathrm{d}q_2 \exp(-ix_1k_1 - ix_2k_2)\mathrm{d}x_1\mathrm{d}x_2 \\ &= q_j \int_{\mathbb{R}^2}\int_{\mathbb{R}^2} Kw_j(\phi, \phi', p_1, p_2)U(q_1, q_2, t)\exp(-i(q_1+p_1)k_1 - i(q_2+p_2)k_2)\mathrm{d}q_1\mathrm{d}q_2\mathrm{d}p_1\mathrm{d}p_2 \\ &= q_j \int_{\mathbb{R}^2} U(q_1, q_2, t)\exp(-iq_1k_1 - iq_2k_2)\mathrm{d}q_1\mathrm{d}q_2 \int_{\mathbb{R}^2} Kw_j(\phi, \phi', p_1, p_2)\exp(-ip_1k_1 - ip_2k_2)\mathrm{d}p_1\mathrm{d}p_2 \\ &= q_j\widehat{Kw_j}(\phi, \phi', k_1, k_2)\hat{U}(k_1, k_2, t) \end{aligned} \tag{1.21}$$

Then we can use inverse Fourier transform to find Turning function

$$T_j\left(\phi, \phi', x_1, x_2\right) = \int_{\mathbb{R}^2} \hat{T}_j\left(\phi, \phi', k_1, k_2\right)\exp(ix_1k_1 + ix_2k_2)\mathrm{d}k_1\mathrm{d}k_2 \tag{1.22}$$

With known turning function, the saturation function can be applied and finally, calculate the interaction term with the most updated density $u(\phi, \phi', X, t)$.

1.4 Applying EDT to the Interaction Term

This section will show how to apply the ETD scheme to the interaction term, which is the non-linear part in the equation.

$$N(u(t),t) = -\lambda(\phi, x_1, x_2)u\left(\phi, x_1, x_2, t\right) + \int_{\phi'=-\pi}^{\pi} S\Big(T\left(\phi, \phi', x_1, x_2\right)\Big)\, u\left(\phi', x_1, x_2, t\right) \mathrm{d}\phi' \tag{1.23}$$

Similar to the transportation term, to apply the ETD method, we need to transform the interaction term into Fourier space over the space variable (x_1, x_2), which can be written as

$$\hat{N}_{k_1,k_2}(t) = \alpha \int_{x_2=-\pi}^{\pi} \int_{x_1=-\pi}^{\pi} N\left(\phi, x_1, x_2, t\right) \exp\left(-i\left[k_1 x_1 + k_2 x_2\right]\right) \mathrm{d}x_1 \ \mathrm{d}x_2 \tag{1.24}$$

Then the equation in the Fourier space becomes

$$\frac{\partial \hat{u}_{k_1,k_2}(\phi,t)}{\partial t} + i\gamma\left[k_1\cos(\phi) + k_2\sin(\phi)\right]\hat{u}_{k_1,k_2}(\phi,t) = \hat{N}_{k_1,k_2}(t) \tag{1.25}$$

which can be approximated by set an intergrating factor $\mu = \exp(-Mt)$ where the matrix M is the same matrix in (1.9). Then the system becomes

$$\frac{\mathrm{d}}{\mathrm{d}t}(\exp(-Mt)\hat{u}) = \exp(-Mt)\hat{N}_{k_1,k_2}(t) \tag{1.26}$$

Then if we integrate both sides over the current time step $t\prime$ and the new time step $t\prime + \Delta t$, the equation becomes

$$\exp(-M[t+\Delta t])\hat{u}(t+\Delta t) - \exp(-Mt)\hat{u}(t) = \int_{t'=t}^{t+\Delta t} \exp\left(-Mt'\right)\hat{N}_{k_2,k_2}\left(t'\right) \mathrm{d}t' \tag{1.27}$$

To approximate the non-linear term, one thing is to make the assumption that the function $\hat{N}_{k_1,k_2}(t) = \hat{N}_{k_1,k_2} + \mathcal{O}(\Delta t)$, which is a constant value of the interaction term at a specific time t. Then the integration part can be calculated as

$$\begin{aligned}\int_{t'=t}^{t+\Delta t} \exp\left(-Mt'\right)\hat{N}_{k_1,k_2}\left(t'\right)\mathrm{d}t' &= \int_{t'=t}^{t+\Delta t} \exp\left(-Mt'\right)\hat{N}_{k_1,k_2}\mathrm{d}t' + \mathcal{O}(\Delta t) \\ &= -M^{-1}\Big(\exp(-M(t+\Delta t)) - \exp(-M(t))\Big)\hat{N}_{k_1,k_2} + \mathcal{O}(\Delta t)\end{aligned}$$

If the result is substitute into (1.27), then

$$\hat{u}(t+\Delta t) = \exp(M\Delta t)\hat{u} + M^{-1}(\exp(M\Delta t) - \mathbb{I})\hat{N}_{k_1,k_2} + \mathcal{O}(\Delta t) \tag{1.28}$$

To simplify the expression, we can define two diagonal matrices A and B so that the diagonal entries are

$$A_{j,j} = \exp\Big(-i\gamma\Delta t\left[k_1\cos(\phi_j) + k_2\sin(\phi_j)\right]\Big) \tag{1.29}$$

$$B_{j,j} = \frac{\exp\left(-i\gamma\Delta t[k_1 cos(\phi_j) + k_2 sin(\phi_j)]\right) - 1}{-i\gamma[k_1 cos(\phi_j) + k_2 sin(\phi_j)]} \tag{1.30}$$

To avoid dividing by 0 when $k_1, k_2 = 0$ in matrix B, we multiply the entry by 1 in the form of

$$\begin{aligned} c_{j,j} &= \exp(\frac{-\Delta t}{2}M_{j,j})^{-1}\exp(\frac{-\Delta t}{2}M_{j,j}) \\ &= \frac{\exp\left(\frac{i}{2}\gamma\Delta t[k_1cos(\phi_j)+k_2sin(\phi_j)]\right)}{\exp\left(\frac{i}{2}\gamma\Delta t[k_1cos(\phi_j)+k_2sin(\phi_j)]\right)} \end{aligned} \tag{1.31}$$

If we let $Q_{j,j} = -[k_1cos(\phi_j)+k_2sin(\phi_j)]$, then the matrix $B_{j,j}$ can be rewritten as

$$\begin{aligned} B_{j,j} &= \frac{\exp\left(-i\gamma\Delta tQ_{j,j}\right)-1}{-i\gamma Q_{j,j}}\cdot\frac{\exp\left(\frac{i}{2}\gamma\Delta tQ_{j,j}\right)}{\exp\left(\frac{i}{2}\gamma\Delta tQ_{j,j}\right)} \\ &= \Delta t\,\mathrm{sinc}(\frac{1}{2}\gamma\Delta tQ_{j,j})\exp(\frac{i}{2}\gamma\Delta tQ_{j,j}) \end{aligned} \tag{1.32}$$

with the sinc function

$$\begin{aligned} \mathrm{sinc}(\frac{1}{2}\gamma\Delta tQ_{j,j}) &= \frac{\sin(\frac{1}{2}\gamma\Delta tQ_{j,j})}{\frac{1}{2}\gamma\Delta tQ_{j,j}} \\ &= \frac{\exp\left(\frac{i}{2}\gamma\Delta tQ_{j,j}\right)-\exp\left(-\frac{i}{2}\gamma\Delta tQ_{j,j}\right)}{i\gamma\Delta tQ_{j,j}} \end{aligned} \tag{1.33}$$

Then finally, we can find the density function in Fourier space $\hat{u}_{k_1,k_2}(t+\Delta t)$ by

$$\hat{u}_{\phi,k_1,k_2}(t+\Delta t) \approx A\hat{u}_{\phi,k_1,k_2}(t) + B\hat{N}_{\phi,k_1,k_2}(t) \tag{1.34}$$

Finally, the density function at new time step $u(\phi,x_1,x_2,t+\Delta t)$ can be calculated by Inverse Fourier Transform

$$u(\phi,x_1,x_2,t+\Delta t) = \frac{1}{N^2}\sum_{k_1=-\frac{N}{2}}^{\frac{N}{2}}\sum_{k_2=-\frac{N}{2}}^{\frac{N}{2}}\hat{u}_{k_1,k_2}(\phi,t)\exp\left(i\left[k_1x_1+k_2x_2\right]\right) \tag{1.35}$$