Spectral Method for Solving PDEs

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$$\frac{\partial \phi}{\partial t} = f\left(\phi, \frac{\partial \phi}{\partial x}, \frac{\partial^2 \phi}{\partial x^2}, t\right)$$

PDEs

- Diffusion eqn
- Wave eqn
- Burgers eqn
- Navier-Stokes equation
- Schrodinger equation
-

Diffusion equation

Diffusion equation

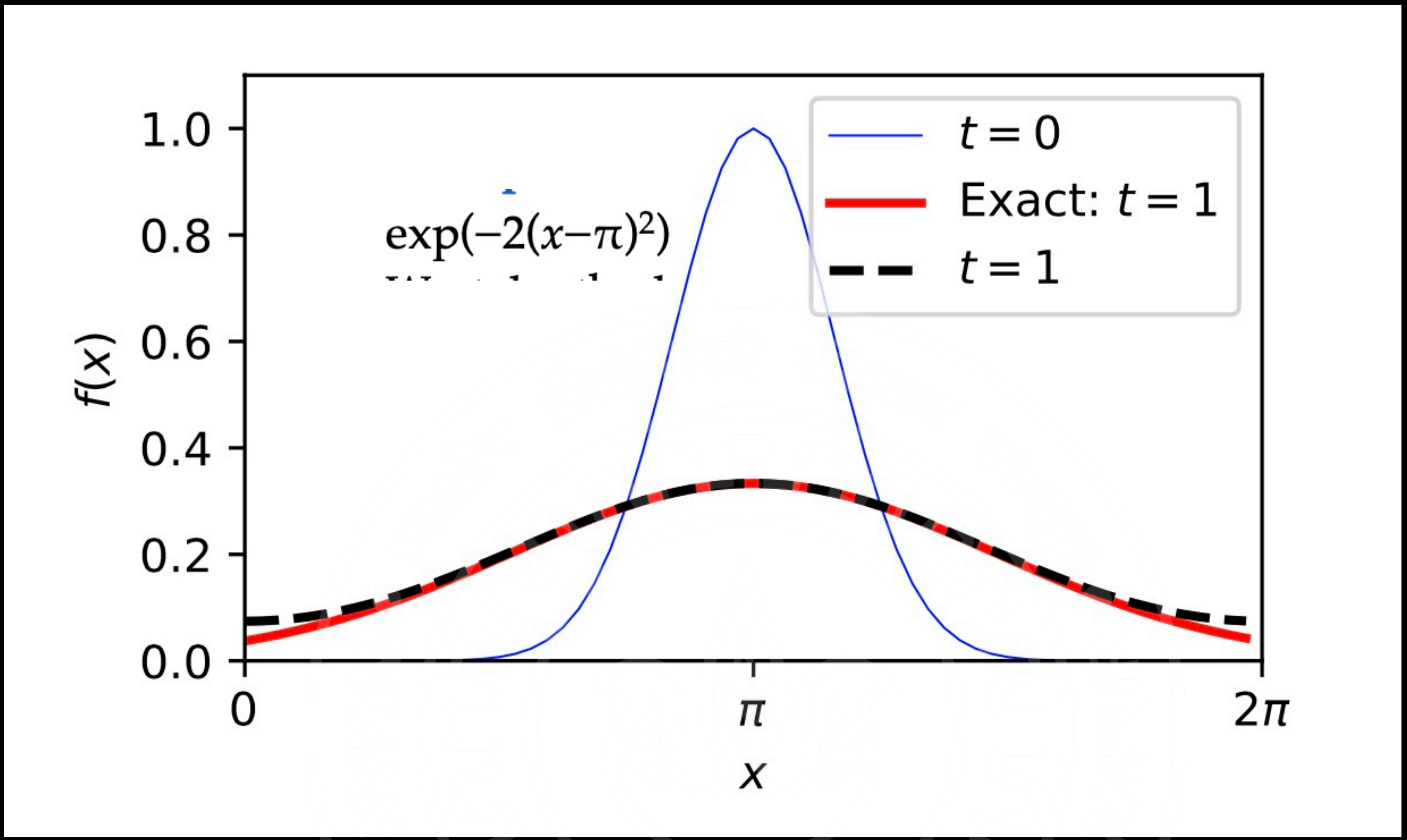
$$\partial_t \phi = \kappa \frac{\partial^2 \phi}{\partial x^2},$$

$$\partial_t \hat{\phi}_k = -\kappa k^2 \hat{\phi}_k,$$

```
kappa = 1; tf = 1
L = 2*np.pi; N = 64; h = L/N
j = np.arange(0,N); x = j*h

f = np.exp(-2*(x-pi)**2)  # init cond
fk = np.fft.rfft(f,N)/N
kx = np.linspace(0, N//2, N//2+1)

# Final states
fk_t = fk*np.exp(-kappa*kx**2*tf)
f_t = np.fft.irfft(fk_t,N)*N  # in Real space
```



t = 0
Exact: t = 1
t = 1
exp(−2(x−π)²)
f(x)
x
1.0
0.8
0.6
0.4
0.2
0.0
0
π
2π

CFL condition

$$\partial_t \hat{\phi}_k = -\kappa k^2 \hat{\phi}_k,$$

$$\hat{\phi}_k^{(n+1)} = \hat{\phi}_k^{(n)}[1 - \kappa k^2(\Delta t)].$$

$$|1 - \kappa k^2(\Delta t)| < 1, \quad \text{or} \quad \Delta t < \frac{2}{\kappa k^2}.$$

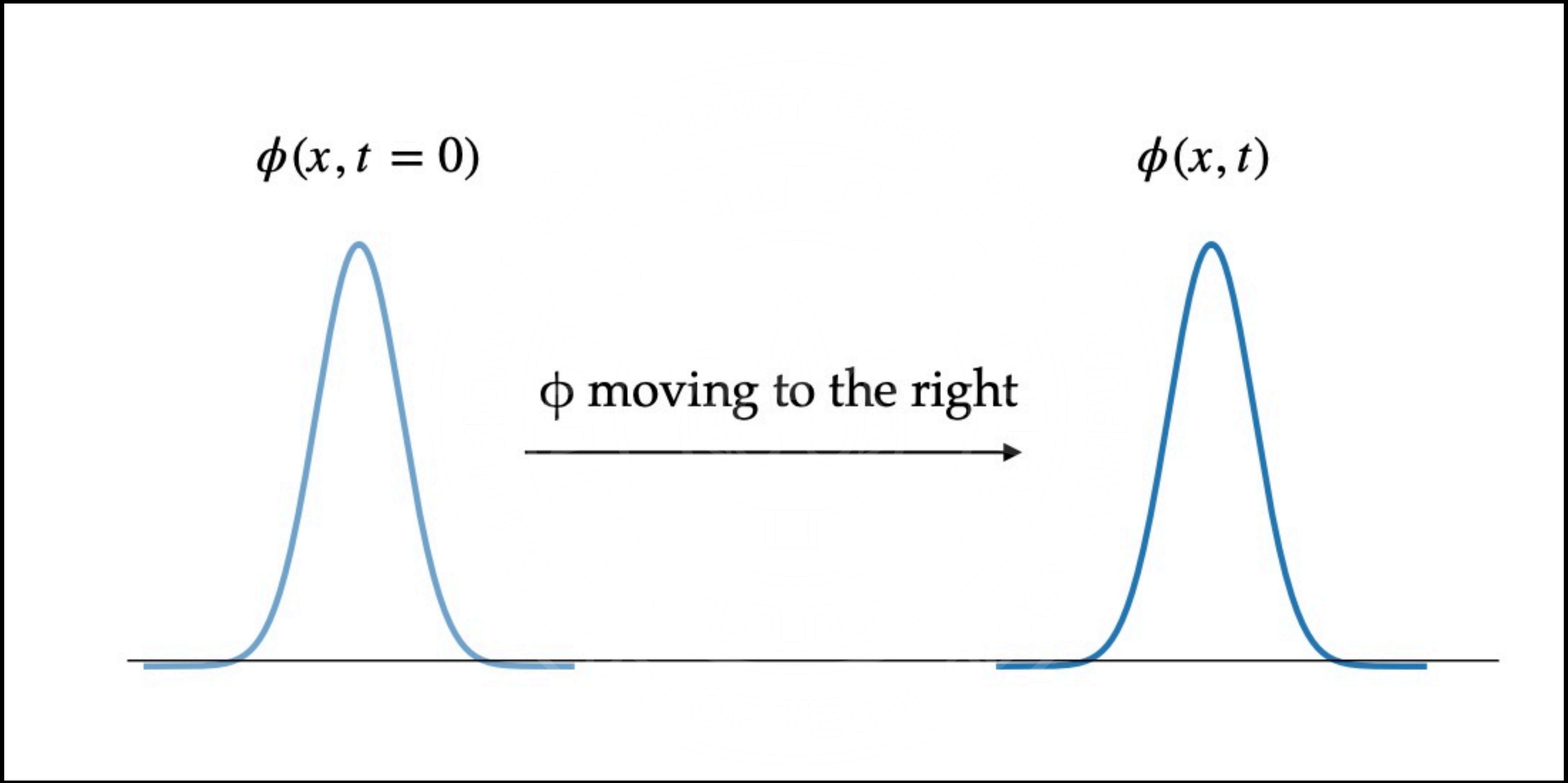
$$\Delta t < \frac{2}{\kappa k_{\text{max}}^2}.$$

$$\Delta t < \frac{2h^2}{\kappa \pi^2}.$$

Wave equation

$$\partial_t \phi + c \partial_x \phi = 0\,,$$

$$\frac{d}{dt}\hat{\phi}_k = -ick\hat{\phi}_k.$$



$\phi(x, t = 0)$
$\phi(x, t)$
ϕ moving to the right

Stability

$$\frac{d}{dt}\hat{\phi}_k = -ick\hat{\phi}_k.$$

$$\hat{\phi}_k^{(n+1)} = (1 - ick(\Delta t))\hat{\phi}_k^{(n)}$$

Burgers equation

$$\partial_t u + u\partial_x u = \nu\, \partial^2 u, \quad \text{or } \partial_t u + \partial_x(u^2/2) = \nu\, \partial_x{}^2 u\ ,$$

$$\frac{d}{dt}\hat{u}_k = -\,i\,\frac{k}{2}\,\widehat{u^2} - \nu k^2 \hat{u}_k = -\,\hat{N}_k - \nu k^2 \hat{u}_k,$$

$$\hat{u}_k^{(n+1)} = \hat{u}_k^{(n)}[1 - \nu k^2(\Delta t)] - (\Delta t)\hat{N}_k.$$

$$|1 - \nu k^2\,(\Delta t)| < 1, \quad \text{or } \Delta t < 2/(\nu k^2).$$

Crank-Nicolson scheme

$$\frac{d}{dt}\hat{u}_k = -i\frac{k}{2}\widehat{u^2} - \nu k^2 \hat{u}_k = -\hat{N}_k - \nu k^2 \hat{u}_k,$$

$$\hat{u}_k^{(n+1)} = \hat{u}_k^{(n)} - \nu k^2 (\Delta t)\frac{1}{2}\left(\hat{u}_k^{(n)} + \hat{u}_k^{(n+1)}\right) - (\Delta t)\hat{N}_k\,,$$

$$\text{or,}\quad \hat{u}_k^{(n+1)} = \hat{u}_k^{(n)}\left[\frac{1 - \nu k^2(\Delta t)/2}{1 + \nu k^2(\Delta t)/2}\right] - (\Delta t)\hat{N}_k$$

Exponential Trick

$$\frac{d}{dt}\hat{u}_k = -i\frac{k}{2}\widehat{u^2} - \nu k^2 \hat{u}_k = -\hat{N}_k - \nu k^2 \hat{u}_k,$$

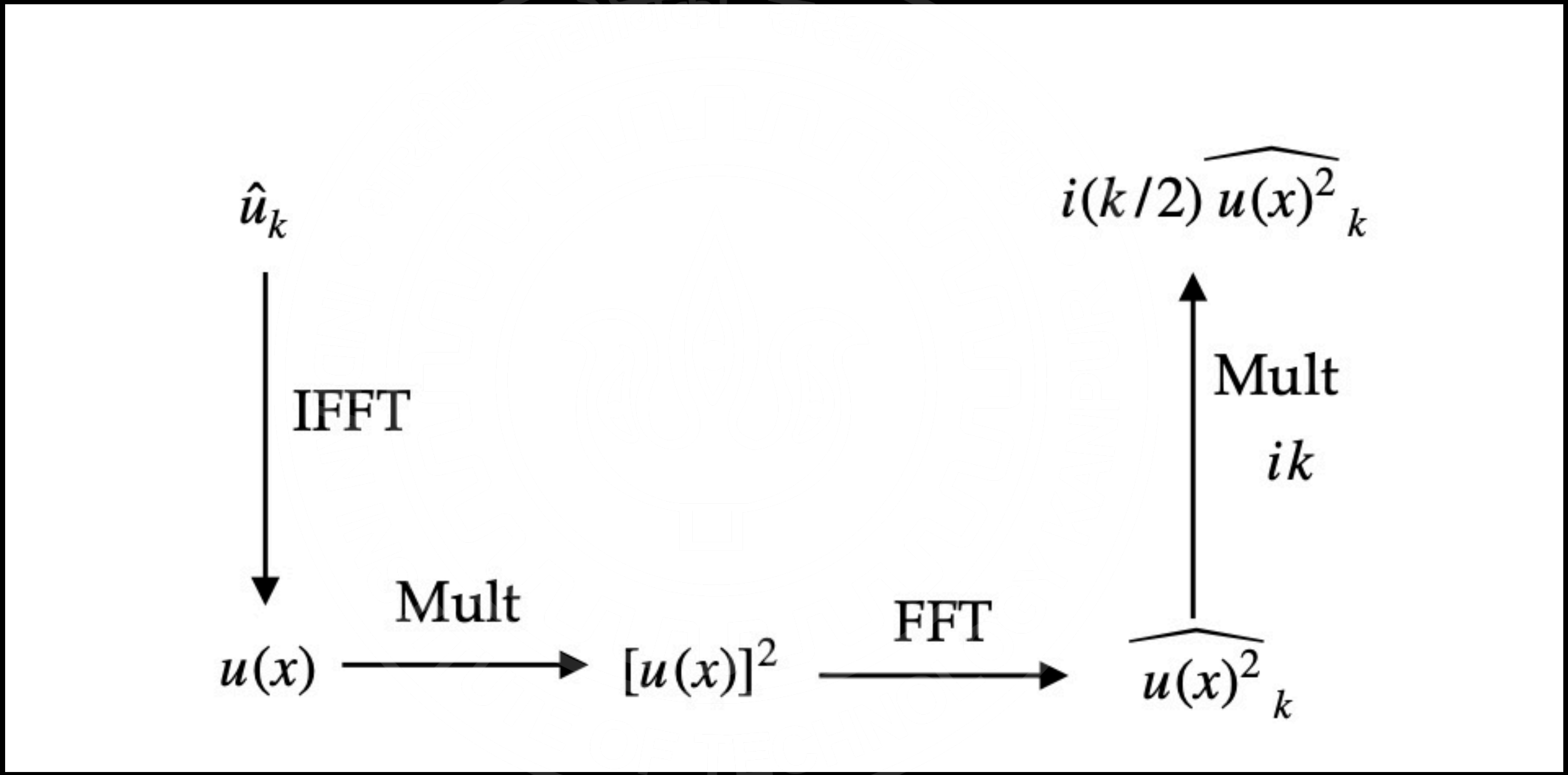
$$\hat{u}'_k = \hat{u}_k \exp(\nu k^2 t),$$

$$\frac{d}{dt}\hat{u}'_k = -\hat{N}_k \exp(\nu k^2 t)\,.$$

An application Euler's forward scheme to the above equation yields

$$\hat{u}_k^{(n+1)} = \left[\hat{u}_k^{(n)} - (\Delta t)\hat{N}_k^{(n)}\right] \exp(-\nu k^2 (\Delta t))\,.$$

Convolution computation



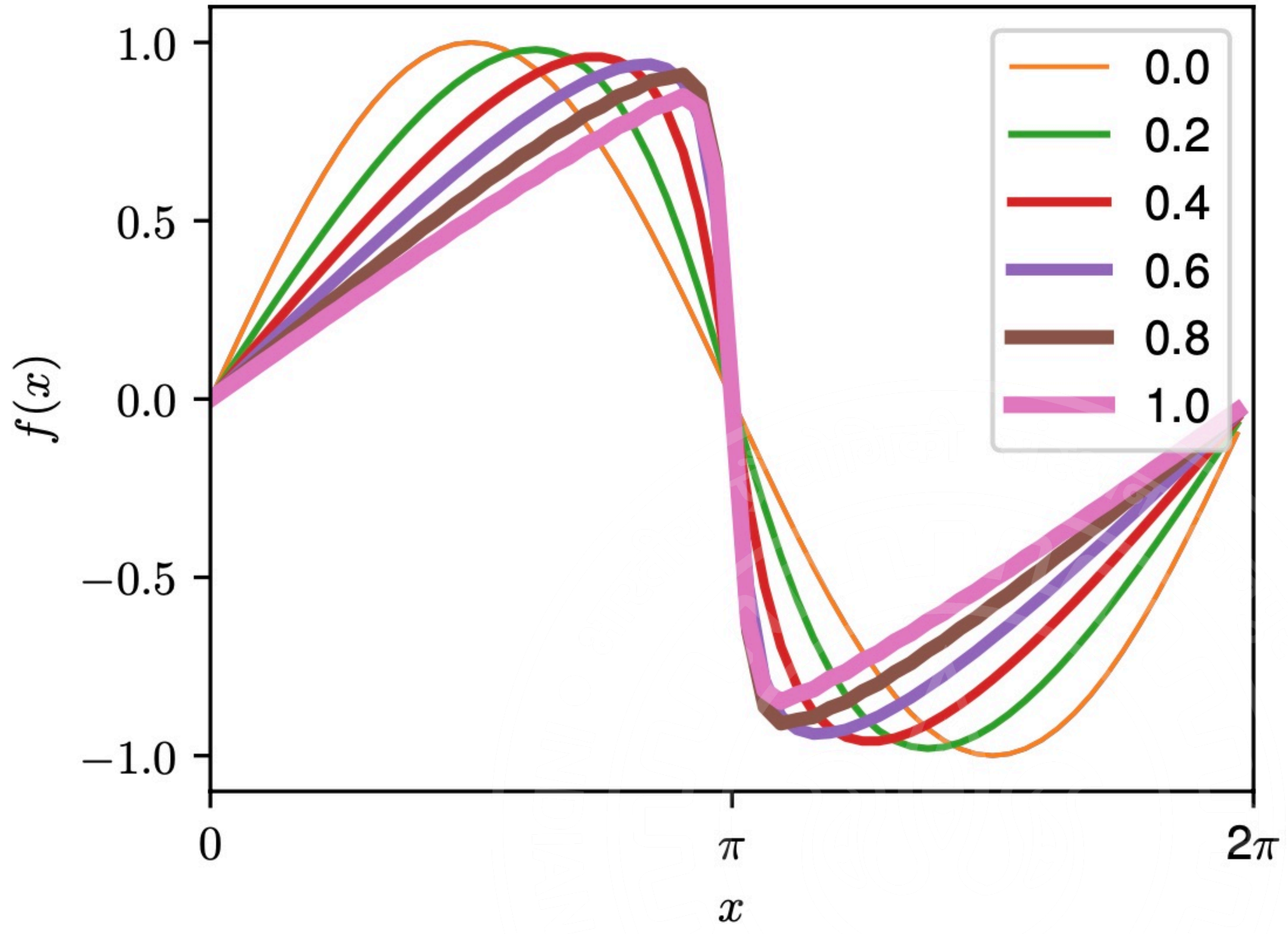
```
nu = 0.1; tf = 1; dt = 0.001; nsteps = int(tf/dt)
L = 2*np.pi; N = 64; h = L/N
j = np.arange(0,N); x = j*h

kx = np.linspace(0, N//2, N//2+1)
exp_factor_dtby2 = np.exp(-nu*kx**2*dt/2)
exp_factor = np.exp(-nu*kx**2*dt)

def comput_Nk(fk):
f = np.fft.irfft(fk,N)*N
    f = f*f
    fk_prod = np.fft.rfft(f,N)/N
    return (1j*kx*fk_prod)

f = np.sin(x) # initiation condition
fk = np.fft.rfft(f,N)/N  # FT(f)
```

```
for i in range(nsteps+2):
    Nk = comput_Nk(fk)
    fk_mid = (fk -(dt/2)*Nk)*exp_factor_dtby2
    Nk_mid = comput_Nk(fk_mid)
    fk = (fk -dt*Nk_mid)*exp_factor
```



$$(\Delta t)_{\min} = \frac{2h^2}{\nu \pi^2} = \frac{2 \times 4\pi^2}{0.1 \times 64^2 \pi^2} = \frac{10}{512} \approx 2 \times 10^{-2} \,.$$

On the other hand, based on the nonlinear term,

$$\Delta t < h/\mathrm{U_{rms}} \approx 1/64 \approx 0.015 \,.$$

$\Delta t = 0.001,$

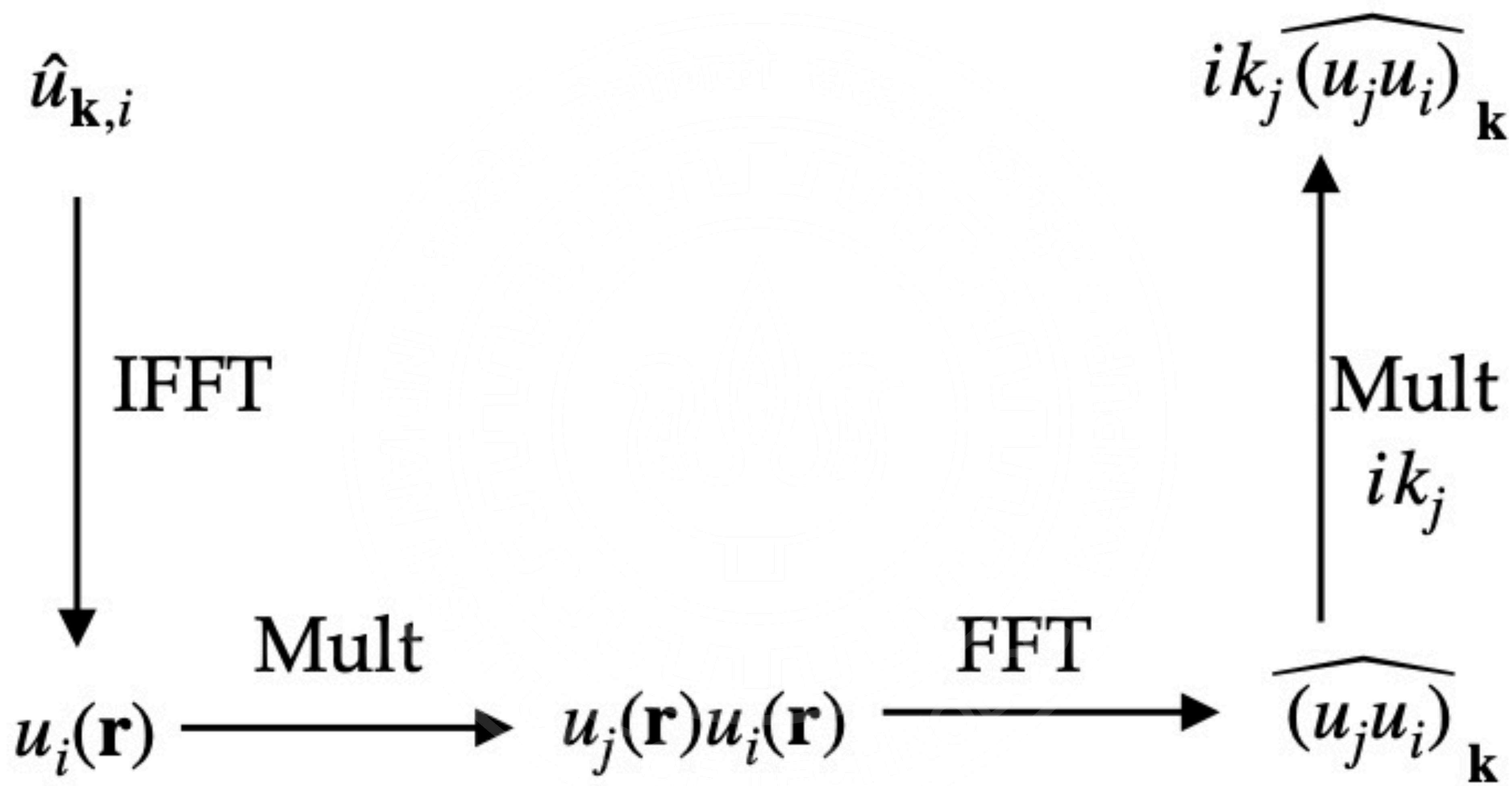
Navier-Stokes eqn

$$\partial_t \mathbf{u} + \mathbf{u} \cdot \nabla \mathbf{u} = -\nabla p + \nu \nabla^2 \mathbf{u}, \quad .....(80)$$

$$\nabla \cdot \mathbf{u} = 0, \quad .....(81)$$

$$\frac{d}{dt}\hat{u}_{\mathbf{k},i} = -i k_j \widehat{u_j(\mathbf{r}) u_i(\mathbf{r})}_{\mathbf{k}} - i k_i \hat{p}_{\mathbf{k}} - \nu k^2 \hat{u}_{\mathbf{k},i}$$
$$= -\hat{N}_{\mathbf{k},i} - i k_i \hat{p}_{\mathbf{k}} - \nu k^2 \hat{u}_{\mathbf{k},i}, \quad .....(82)$$

$$k_i \hat{u}_{\mathbf{k},i} = 0.$$


$\hat{u}_{\mathbf{k},i}$
IFFT
$u_i(\mathbf{r})$
Mult
$u_j(\mathbf{r})u_i(\mathbf{r})$
FFT
$\widehat{(u_j u_i)}_{\mathbf{k}}$
Mult
ik_j
$ik_j \widehat{(u_j u_i)}_{\mathbf{k}}$

Pressure computation

$$\partial_t \mathbf{u} + \mathbf{u} \cdot \nabla \mathbf{u} = -\nabla p + \nu \nabla^2 \mathbf{u}, \quad .....(80)$$

$$\nabla \cdot \mathbf{u} = 0, \quad .....(81)$$

$$-\nabla^2 p = \nabla \cdot [\mathbf{u} \cdot \nabla \mathbf{u}] = \nabla \cdot \mathbf{N},$$

$$\hat{p}_{\mathbf{k}} = i \frac{1}{k^2} \mathbf{k} \cdot \hat{\mathbf{N}}_{\mathbf{k}},$$

$$\frac{d}{dt} \hat{u}_{\mathbf{k},i} = -i k_j \widehat{u_j(\mathbf{r}) u_i(\mathbf{r})}_{\mathbf{k}} - i k_i \hat{p}_{\mathbf{k}} - \nu k^2 \hat{u}_{\mathbf{k},i}$$
$$= -\hat{N}_{\mathbf{k},i} - i k_i \hat{p}_{\mathbf{k}} - \nu k^2 \hat{u}_{\mathbf{k},i}, \quad .....(82)$$

$$\hat{\mathbf{u}}_{\mathbf{k}}^{(n+1)} = \hat{u}_{\mathbf{k}}^{(n)}[1 - \nu k^2 (\Delta t)] + (\Delta t)[-\hat{N}_{\mathbf{k}} - i \mathbf{k} \hat{p}_{\mathbf{k}}^{(n)}]$$

$$\frac{d}{dt}\hat{u}_{\mathbf{k},i} = -ik_j \widehat{u_j(\mathbf{r})u_i(\mathbf{r})}_{\mathbf{k}} - ik_i\hat{p}_{\mathbf{k}} - \nu k^2 \hat{u}_{\mathbf{k},i}$$

$$= -\hat{N}_{\mathbf{k},i} - ik_i\hat{p}_{\mathbf{k}} - \nu k^2 \hat{u}_{\mathbf{k},i}, \quad .....(82)$$

$$\Delta t < \tau_\nu = \frac{2h^2}{\nu \pi^2}.$$

$$\tau_{\mathrm{NL}} = h/\mathbf{u}_{\mathrm{rms}}.$$

$$\tau_\nu / \tau_{\mathrm{NL}} \approx u_{\mathrm{rms}} h/\nu \approx \mathrm{Re}/N,$$

$$\frac{\tau_\nu}{\tau_{NL}} \approx \frac{u_{\mathrm{rms}} h}{\nu} \approx \frac{\mathrm{Re}}{N} \approx \frac{\mathrm{Re}}{\mathrm{Re}^{3/4}} \approx \mathrm{Re}^{1/4}.$$

Schrödinger Equaion

$$i\hbar\partial_t\psi = \left[-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r})\right]\psi\,,$$

$t = t'(\hbar/E_a)$ and $\mathbf{r} = \mathbf{r}'r_a$,

$$i\partial_{t'}\psi = \left[-\frac{\alpha}{2}\nabla'^2 + V'(\mathbf{r}')\right]\psi\,,$$

$\alpha = \hbar^2/(\mathrm{m}r_a{}^2E_a)$ and $V'=V/E_a$.

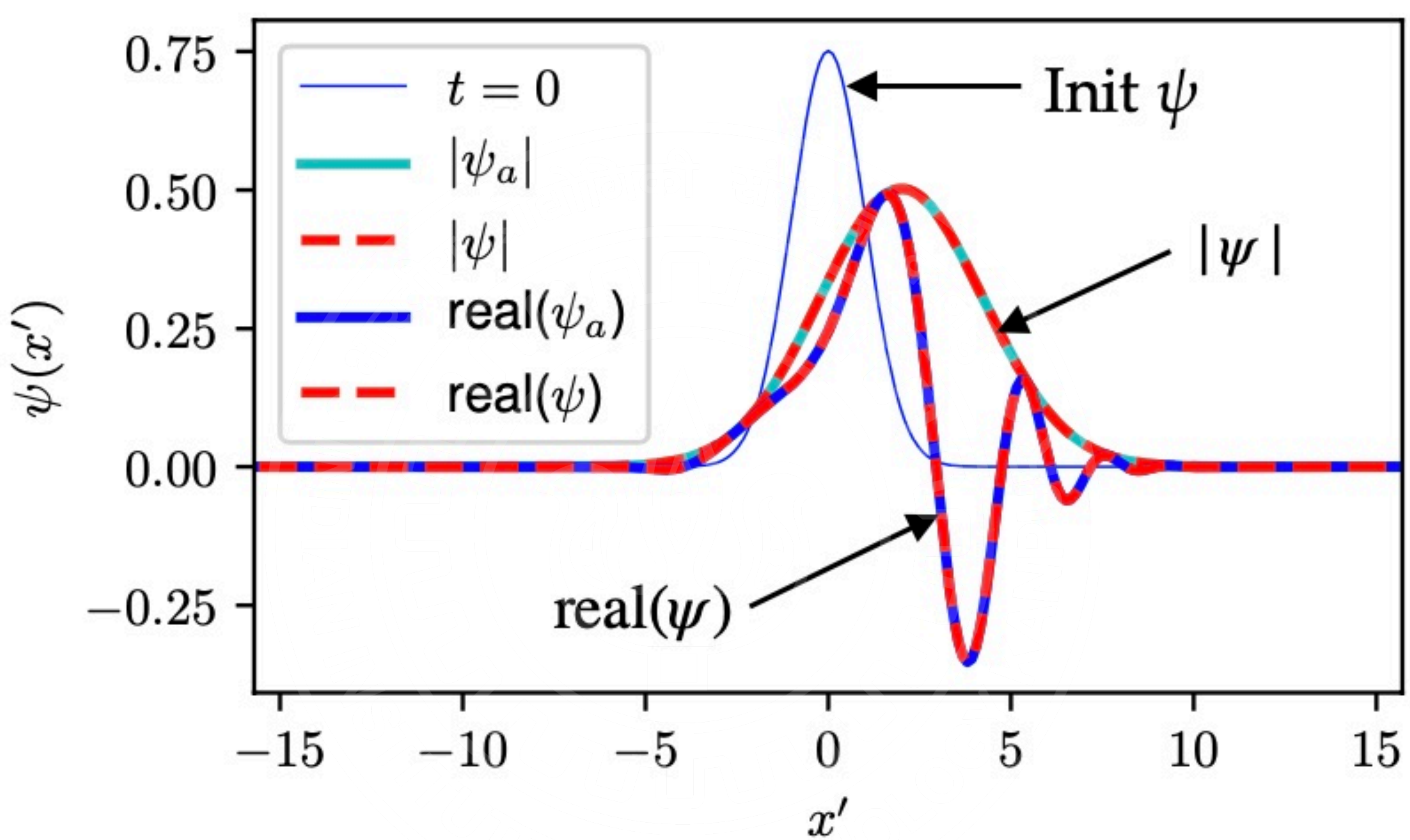
$$\partial_{t'}\hat{\psi}_{\mathbf{k}'} = -i\,\frac{\alpha}{2}k'^2\hat{\psi}_{\mathbf{k}'} - i\,\widehat{(V'\psi)}_{\mathbf{k}'}\,,$$

$$\partial_{t'}\hat{\psi}_{\mathbf{k}'} = -\,i\,\frac{\alpha}{2}k'^2\hat{\psi}_{\mathbf{k}'} - i\,\widehat{(V'\psi)}_{\mathbf{k}'}\,,$$

$$\tilde{\hat{\psi}}_{\mathbf{k}'} = \hat{\psi}_{\mathbf{k}'}\exp(i\,\frac{\alpha}{2}k'^2 t').$$

$$\partial_{t'}\tilde{\hat{\psi}}_{\mathbf{k}'} = -\,i\,\widehat{(V'\psi)}_{\mathbf{k}'}\exp(i\,\frac{\alpha}{2}k'^2 t')\,.$$

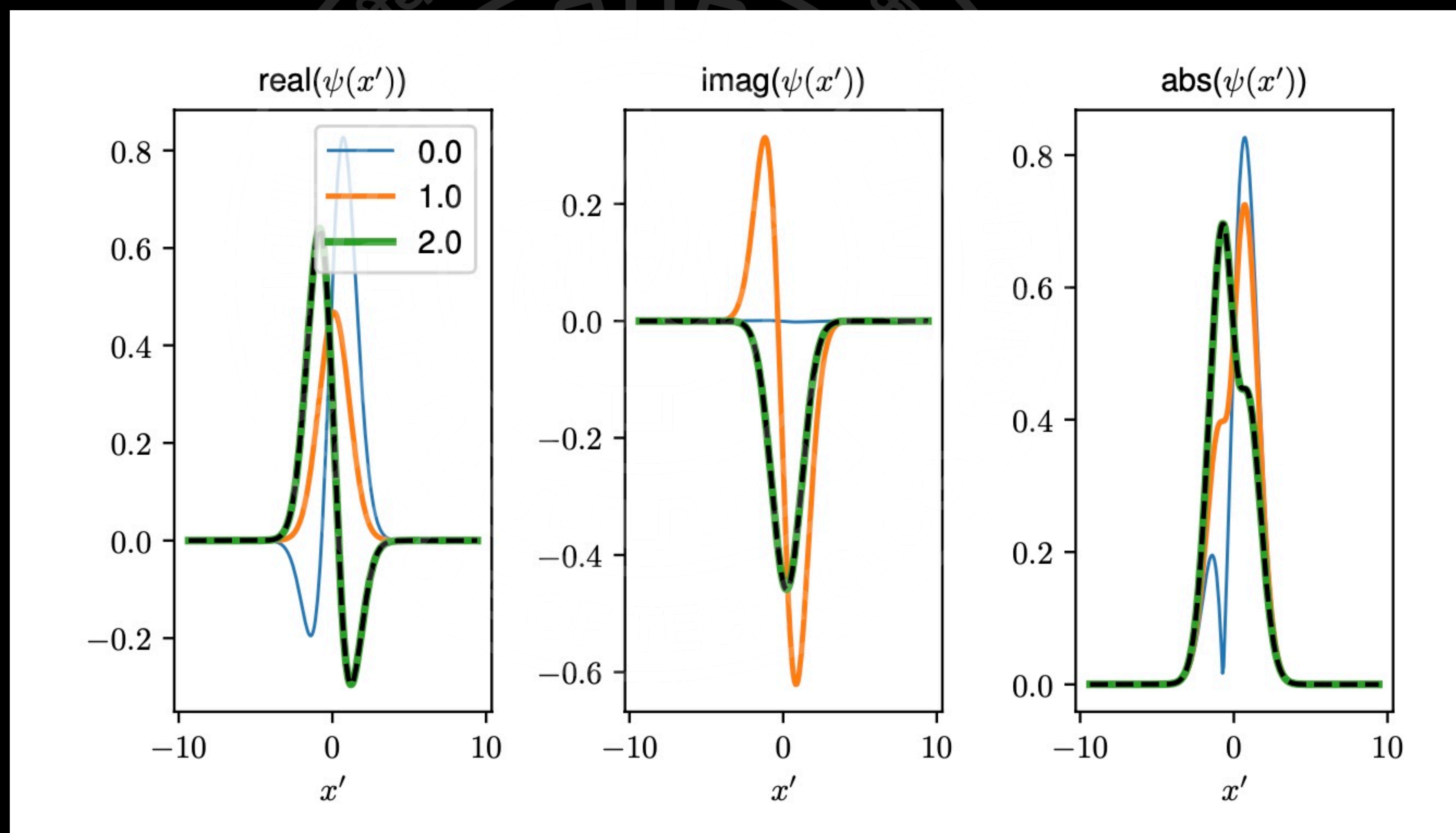
$$\hat{\psi}^{(n+1)}_{\mathbf{k}'} = \hat{\psi}^{(n-1)}_{\mathbf{k}'}\exp(-i\,\alpha\,k'^2(\Delta t')) - i(2\Delta t')\widehat{(V'\psi)}_{\mathbf{k}'}\exp(-i\,\frac{\alpha}{2}k'^2(\Delta t'))$$



0.75
0.50
0.25
0.00
−0.25
$\psi(x')$
$t = 0$
$|\psi_a|$
$|\psi|$
real(ψ_a)
real(ψ)
Init ψ
$|\psi|$
real(ψ)
−15
−10
−5
0
5
10
15
x'

Quantum Oscillator

$$i\partial_{t'}\psi = -\frac{1}{2}\frac{d^2\psi}{dx'^2} + \frac{1}{2}x'^2\psi\,.$$



Gross–Pitaevskii Equation

$$i\hbar\partial_t\psi = \left[-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r}) + g\,|\psi\,|^2\right]\psi\,,$$

$$i\hbar\partial_t\hat{\psi}_{\mathbf{k}} = \frac{\hbar^2 k^2}{2m}\hat{\psi}_{\mathbf{k}} + \widehat{(V\psi)}_{\mathbf{k}} + (g\,\widehat{|\psi\,|^2\psi})_{\mathbf{k}}\,,$$

Thank you!