$\boxed{dk}$ $dk = 2\pi/(b-a)$ $\boxed{2\pi/(N*dx)}$.

$\boxed{k0}$ If no input value given

$$k0 = -\frac{N \times dk}{2}$$

$$\boxed{\begin{aligned} &= -\frac{N}{2} * \frac{2\pi}{N*dx} \\ &= \pi/dx \end{aligned}}$$

$\boxed{k}$ $k = [k0,\ k0+dk,\ k0+2dk, \dots,\ k0+(N-1)dk]$

$$\boxed{= \left[\pi/dx,\ \pi/dx + \frac{2\pi}{\underset{\uparrow\, b-a.}{N*dx}},\ \pi/dx + \frac{4\pi}{N*dx}, \dots,\ \frac{\pi}{dx} + \frac{(N-1)2\pi}{N*dx}\right]}$$

$\boxed{\Psi}$ $\boxed{psi\_x}$ Initialisation psi_x = psi_x0

$\hat{\Psi}$

$$psi\_x = \left[e^{ik[0]*x} * \frac{(2\pi)^{\frac{1}{2}}}{dx}\right] * \_psi\_discrete\_x$$

Ψ

$$psi\_x = \left[e^{ik[0]*x} * \frac{(2\pi)^{\frac{1}{2}}}{dx}\right] * \_psi\_discrete\_x.$$

$$= \frac{(2\pi)^{\frac{1}{2}}}{dx} \left[e^{ik_0 x[0]} * \hat{\Psi}[0], e^{ik_0 x[1]} * \hat{\Psi}[1], \ldots, e^{ik_0 x[N-1]} * \hat{\Psi}[N-1] \right]$$

$\boxed{\hat{\Psi}}$ $\boxed{\text{psi\_discrete\_x}}$

$$\hat{\Psi} = \Psi * e^{-i * k_0 * x} * \frac{dx}{(2\pi)^{\frac{1}{2}}}$$

$$= \frac{dx}{(2\pi)^{\frac{1}{2}}} \left[e^{-ik_0 x[0]} \Psi[0], e^{-ik_0 x[1]} \Psi[1], \ldots, e^{ik_0 x[N-1]} \Psi[N-1] \right]$$

$$= \left[\hat{\Psi}[0], \hat{\Psi}[1], \ldots, \hat{\Psi}[N-1] \right]$$

$\boxed{\text{\_get\_dt}}$ Returns `_dt`.

$\boxed{\text{\_set\_dt}}$

Takes an in_value_dt.
If different from _dt

- Sets _dt = in_value_dt
- Sets _x_evolve_half $= e^{-\frac{V\_x * \_dt\, i}{2\, hbar}}$

$$= \left[e^{-\frac{V\_x[0] * \_dt\, i}{2\, hbar}}, \ldots, e^{-\frac{V\_x[N-1] * \_dt\, i}{2\, hbar}} \right]$$

$$= \left[e^{\frac{-V\_x[0]\, dt\, i}{2\hbar}}, \ldots, e^{\frac{-V\_x[N-1]\, dt\, i}{2\hbar}} \right]$$

- self._k_evolve = $e^{-\frac{k^{**2} * hbar * dt * i}{2m}}$

$$= \left[e^{-\frac{k[0]^{**2} * hbar * dt * i}{2*m}}, \ldots, e^{-\frac{k[N-1]^{**2} * hbar * dt * i}{2*m}} \right]$$

$$= \left[e^{-\frac{k[0]^2 \hbar \, dt \, i}{2m}}, \ldots, e^{-\frac{[N-1]^2 \hbar \, dt \, i}{2m}} \right]$$

ignored for simplicity

$\boxed{\text{time\_step}}$ Signature : time_step(self, dt, Nsteps = 1)

self.dt = dt.

for i = 0, 1, ..., Nsteps − 1 :

$\boxed{\text{Step 1}}$ $\hat{\Psi} = \hat{\Psi} * \_x\_evolve\_half$

$$= \hat{\Psi} * e^{-\frac{V\_x * dt * i}{2\,hbar}}$$

$$= \left[\hat{\Psi}[0] * e^{-\frac{V\_x[0] * dt * i}{2\,hbar}}, \ldots, \hat{\Psi}[N-1] * e^{-\frac{V\_x[N-1] * dt * i}{2\,hbar}} \right]$$

$$= \left[\hat{\Psi}[0]\, e^{-\frac{V\_x[0]\, dt\, i}{2\hbar}}, \ldots, \hat{\Psi}[N-1]\, e^{-\frac{V\_x[N-1]\, dt\, i}{2\hbar}} \right]$$

$\boxed{\hat{k}}$ $\boxed{\text{psi\_discrete\_k}}$

$\boxed{\text{Step 2}}$ psi_discrete_k = fft($\hat{\Psi}$).

$$\boxed{\text{i.e. } \hat{k} = \text{fft}(\hat{\Psi})}$$

Step 3 $\hat{k} = \hat{k} * \_k\_evolve$

$$= \left[\hat{k}[0] * e^{-\frac{k[0]^2 \hbar \, dt \, i}{2m}}, \ldots, \hat{k}[N-1] * e^{-\frac{[N-1]^2 \hbar \, dt \, i}{2m}} \right]$$

Step 4 $\hat{\Psi} = \mathrm{ifft}(\hat{k})$

Step 5 $\hat{\Psi} = \hat{\Psi} * x\_evolve\_half$

$$= \left[\hat{\Psi}[0] \, e^{-\frac{V\_x[0] \, dt \, i}{2\hbar}}, \ldots, \hat{\Psi}[N-1] \, e^{-\frac{V\_x[N-1] \, dt \, i}{2\hbar}} \right]$$

$t = t + Nsteps * dt$

self.t = self.t + Nsteps * self.dt

gauss_x(x, a, x0, k0)

Returns: $(a * \pi^{\frac{1}{2}})^{-\frac{1}{2}} * e^{-\left(\frac{x - x0}{a}\right)^2 + k0 * x \, i}$

$$= (a \, \pi^{\frac{1}{2}})^{-\frac{1}{2}} \left[e^{-\left(\frac{x[0] - x0}{a}\right)^2 + k0 * x[0] i}, \ldots, e^{-\left(\frac{x[N-1] - x0}{a}\right)^2 + k0 * x[N-1] i} \right]$$

$\boxed{\text{Variables}}$