finite difference time domain (FDTD)
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$$i\hbar\Psi(z,t)t = -\frac{\hbar^2}{2m}\Psi(z,t)z+V(z)\Psi(z,t) \quad (1)$$

$\Psi(z,t) = \Psi_r(z,t)+i\Psi_i(z,t)$

$\hbar\Psi_i(z,t)t = -\frac{\hbar^2}{2m}\Psi_r(z,t)z+V(z)\Psi_r(z,t)$

$\hbar\Psi_r(z,t)t = -\frac{\hbar^2}{2m}\Psi_i(z,t)z+V(z)\Psi_i(z,t)$

$z = s\Delta z$
$t = n\Delta t$
Ψ_r
n
Ψ_i
n
$t = n\Delta t$
$z = s\Delta z$
$\Psi(s,n)$
$\Psi(s\Delta z, n\Delta t)$

$$\hbar\frac{\Psi_i(s,n+0.5)-\Psi_i(s,n-0.5)}{\Delta t} = \frac{\hbar^2}{2m}\frac{\Psi_r(s+1,n)-2\Psi_r(s,n)+\Psi_r(s,n-1)}{(\Delta z)^2}-V(s\Delta z)\Psi_r(s,n) \quad (2)$$

$t = (n+0.5)\Delta t$
$z = s\Delta z$

$\hbar\frac{\Psi_r(s,n+1)-\Psi_r(s,n)}{\Delta t} = -\frac{\hbar^2}{2m}\frac{\Psi_i(s+1,n+0.5)-2\Psi_i(s,n+0.5)+\Psi_i(s-1,n+0.5)}{(\Delta z)^2}+V(s\Delta z)\Psi_i(s,n+0.5)$

$$\Psi_i(s,n+0.5) = \Psi_i(s,n-0.5)+\xi\left[\Psi_r(s+1,n)-2\Psi_r(s,n)+\Psi_r(s,n)\right]-\frac{\Delta t V(s\Delta z)}{\hbar}\Psi_r(s,n) \quad (3)$$

$$\Psi_r(s,n+1) = \Psi_r(s,n)-\xi\left[\Psi_i(s+1,n+0.5)-2\Psi_i(s,n+0.5)+\Psi_i(s,n+0.5)\right]+\frac{\Delta t V(s\Delta z)}{\hbar}\Psi_i(s,n) \quad (4)$$

ξ

$$\xi = \frac{\hbar\Delta t}{2m(\Delta x)^2}$$

$t = 0$
o

$$\Psi(z,t=0) = \left(\frac{2}{\pi\sigma^2}\right)^{\frac{1}{4}}\exp\left(\frac{-(z-z_0)^2}{\sigma^2}\right)\exp\left(\frac{2\pi i(z-z_0)}{\lambda_e}\right) \quad (5)$$

z_0
$z_0 = 0$
λ_e
$\Delta z = 0.1\text{nm}$
$\Delta t = 0.02\text{fs}$
$\sigma =$
$\lambda_e = 5\text{nm}$
nm
fs
em
0.511Mev
$\hbar \approx 0.658\text{eV.fs}$
$V = 0$
$\alpha\ t$

$$\Psi(z,t) = \frac{1}{2\pi\hbar}\int_{-\infty}^{+\infty} dp \int_{-\infty}^{+\infty} dz'\Psi(z',0)\exp\left[\frac{-ip^2t}{2m\hbar}+\frac{ip(z-z')}{\hbar}\right]$$
(11)

$$\Phi(k) = \int_{-\infty}^{+\infty}\Psi(z',0)\exp\left(-ikz'\right)$$
(12)

$$\Phi(k) = \left(\frac{\sigma^2}{2\pi}\right)^{\frac{1}{4}}\exp\left[-\frac{(k-2\pi/\lambda_e)^2\sigma^2}{4}\right]$$
(13)

$z_0 = 0$,

ω

k

$$v_g \approx \left(\omega(k)k\right)_{k=k_0} = \frac{\hbar k_0}{m}$$
(14)

$k_0 = \frac{2\pi}{\lambda_e}$

$k = k_0$

$$\omega(k) \approx \omega(k_0)+(k-k_0)\left(\omega k\right)_{k=k_0}+\frac{1}{2}(k-k_0)^2\left(\omega k\right)_{k=k_0}$$
(15)

$$\hbar\omega = \frac{p^2}{2m}$$

ω

$$\Psi(z,t) \approx \left[\frac{2}{\pi(\sigma^2+4i\gamma t)}\right]^{\frac{1}{4}}\exp i(k_0z-\omega_0t)\exp\left[-\frac{(z-v_gt)}{\sigma^2+4i\gamma t}\right]$$
(16)

$\gamma = \left(\omega k\right)_{k=k_0}$

x

t

$$\Psi(x,t)^2 = \left[\frac{4}{\pi^2\left(\sigma^4+16\gamma^2t^2\right)}\right]^{\frac{1}{4}}\exp\left[-\frac{2\sigma^2(z-v_gt)}{\sigma^2+16\gamma^2t^2}\right]$$

v_g

kinetic energy

$$\langle K\rangle_t = \alpha,t\frac{p^2}{2m}\alpha,t = -\frac{\hbar^2}{2m}\int_{-\infty}^{+\infty}\Psi^*(z,t)\Psi(z,t)z$$
(18)

$\langle K\rangle_{n\Delta t} \approx -\frac{\hbar^2}{2m}\sum_s\Psi^*(s,n)\frac{\Psi(s+1,n)-2\Psi(s,n)+\Psi(s-1,n)}{\Delta z}$

$\Psi(s,n) = \Psi_r(s,n)+i\frac{1}{2}\left[\Psi_i(s,n+0.5)+\Psi_i(s,n-0.5)\right]$

constant of motion

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$$\frac{d\langle K\rangle_t}{dt} = \frac{1}{i\hbar}\left[H,H\right] = 0$$
(19)

$$\langle K\rangle = \int_{-\infty}^{+\infty} dk\frac{\hbar^2k^2}{2m}\Phi(k)^2 = \frac{\sigma\hbar^2}{2m\sqrt{2\pi}}\int_{-\infty}^{+\infty}k^2\exp\left[\frac{1}{2}\sigma^2(k-k_0)^2\right]dk$$
(20)

$$\langle K\rangle = \frac{\hbar^2k_0^2}{2m}+\frac{\hbar^2}{2m\sigma^2} = \frac{1}{2}mv_g^2+\frac{\hbar^2}{2m\sigma^2}$$
(21)

$$\langle K\rangle = K_{classic}+\frac{\hbar^2}{2m\sigma^2}$$
(22)

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$\Psi(r,t)$

??
Ψ^2
$t =$
34fs
$t =$
68fs
$t =$
34fs
$\Psi(r,t)^2$
$t =$
34fs
$t =$
68fs
$\Psi(r,t)^2$
$t =$
68fs