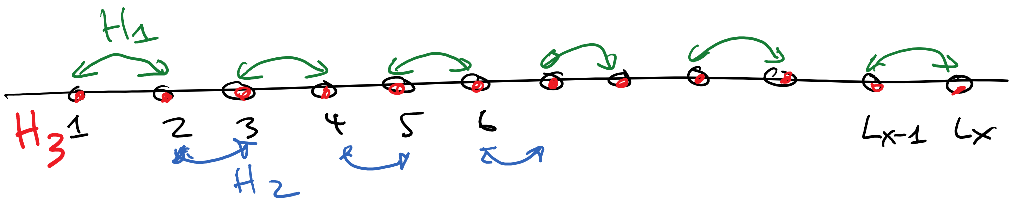
TDSE Implementation Details

Monday, 28 February 2022 07:34

Recall that

$$H = -\frac{1}{4\pi^2\Delta^2}\sum_{\ell=1}^{L_x-1}\left(c_\ell^\dagger c_{\ell+1} + c_{\ell+1}^\dagger c_\ell\right) + \frac{1}{4\pi^2\Delta^2}\sum_{\ell=1}^{L_x}\left(2 + 4\pi^2\Delta^2 V_\ell\right)$$



$$H = H_1 + H_2 + H_3$$

where

$$H_1 = -\frac{1}{4\pi^2\Delta^2}\sum_{\ell=1,3,5,7}^{L_x-1}\left(c_\ell^\dagger c_{\ell+1} + c_{\ell+1}^\dagger c_\ell\right)$$

$$H_2 = -\frac{1}{4\pi^2\Delta^2}\sum_{\ell=2,4,6}^{L_x-1}\left(\cdots\right)$$

$$H_3 = \frac{1}{4\pi^2\Delta^2}\sum_{\ell=1}^{L_x}\left(2 + 4\pi^2\Delta^2 V_\ell\right)$$

Now ~~set~~ set $\quad U_1(\tau) = \prod_{q=1}^{3} e^{-i\tau H_q} \approx e^{-i\tau H}$

1st order approximation

2nd order Method

$$U_2(\tau) = U_1\left(\frac{\tau}{2}\right)U_1^\dagger\left(\frac{\tau}{2}\right)$$

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e.g. $\quad H = T + V$

$$U_1(\tau) = e^{-i\tau T}e^{-i\tau V}$$

$$U_2(\tau) = e^{-i\frac{\tau}{2}T} \underbrace{e^{-i\frac{\tau}{2}V} e^{-i\frac{\tau}{2}V}}_{e^{-i\tau V}} e^{-i\frac{\tau}{2}T}$$

this leapfrog!

$$U_2(\tau) = e^{-i\frac{\tau}{2}H_3} \boxed{e^{-i\frac{\tau}{2}H_2} e^{-i\frac{\tau}{2}H_1} e^{-i\frac{\tau}{2}H_1} e^{-i\frac{\tau}{2}H_2}} \times e^{-i\frac{\tau}{2}H_3}$$

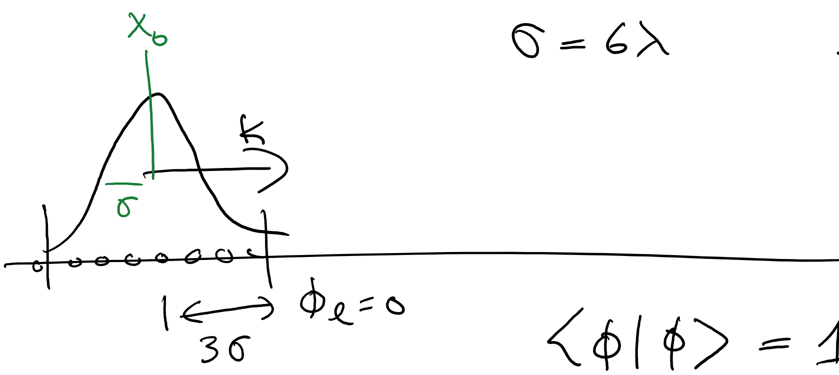
these use M!

Gaussian Wavepacket

$$\phi(x) \propto \frac{1}{\sqrt{\langle\phi|\phi\rangle}} e^{2\pi i k x} e^{-\frac{(x-x_0)^2}{2\sigma^2}}$$

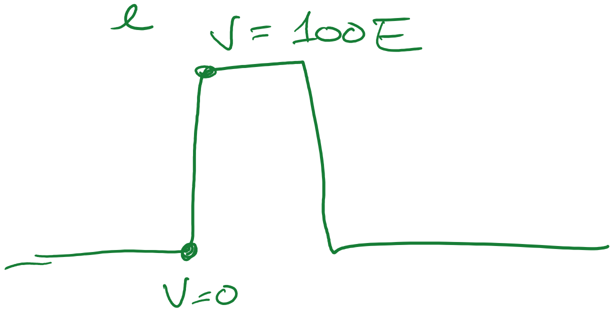
$\lambda = 1$ use $k = 1$

$\sigma = 6\lambda$ $\Delta = 0.1\lambda$

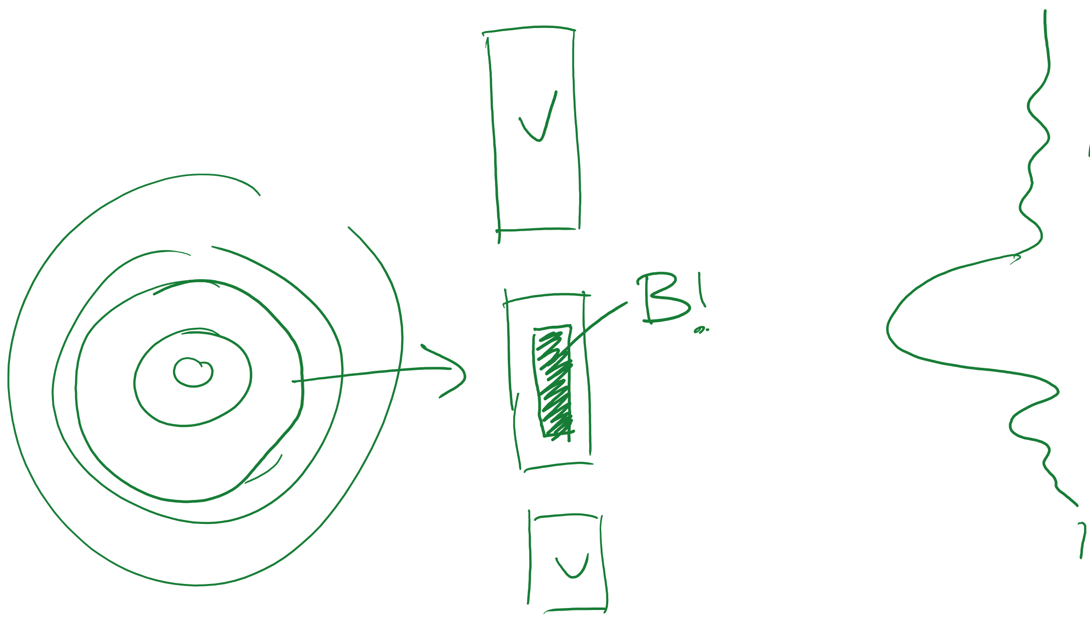


$\langle\phi|\phi\rangle = 1$

$$\langle\phi|\phi\rangle = \sum_\ell \phi_\ell^* \phi_\ell$$



2-D 4th-order → still only need M



Application to Ahranov-Böhm effect.

- using complex time this is also an explicit, stable 2^{nd} order space & time method to solve the diffusion equation! (like implicit Crank-Nicholson method).