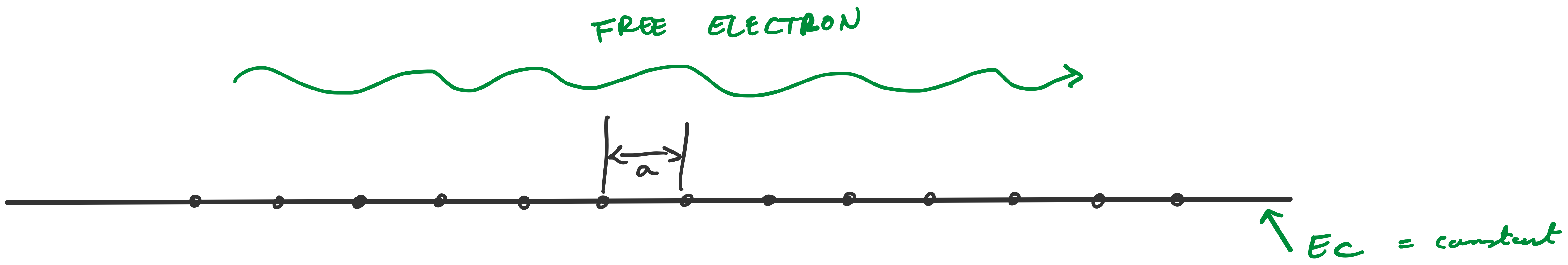
LIMIT OF VALIDATION OF THE EMA

Wednesday, 19 December 2018 14:08



$$-\frac{\hbar^2}{2m^*}\frac{\partial^2\varphi}{\partial x^2} + E_c\varphi = E\varphi$$

in the n-th point, the Schroedinger equation is discretized as:

$$-t_0\left[\varphi_{n+1} - 2\varphi_n + \varphi_{n-1}\right] = (E-E_c)\varphi_n$$

$$\varphi(x) = e^{jkx} \xrightarrow{x=na} \varphi(na) = e^{jkna}$$

$$-t_0\left[e^{jk(n+1)a} - 2e^{jkna} + e^{jk(n-1)a}\right] = (E-E_c)\,e^{jkna}$$

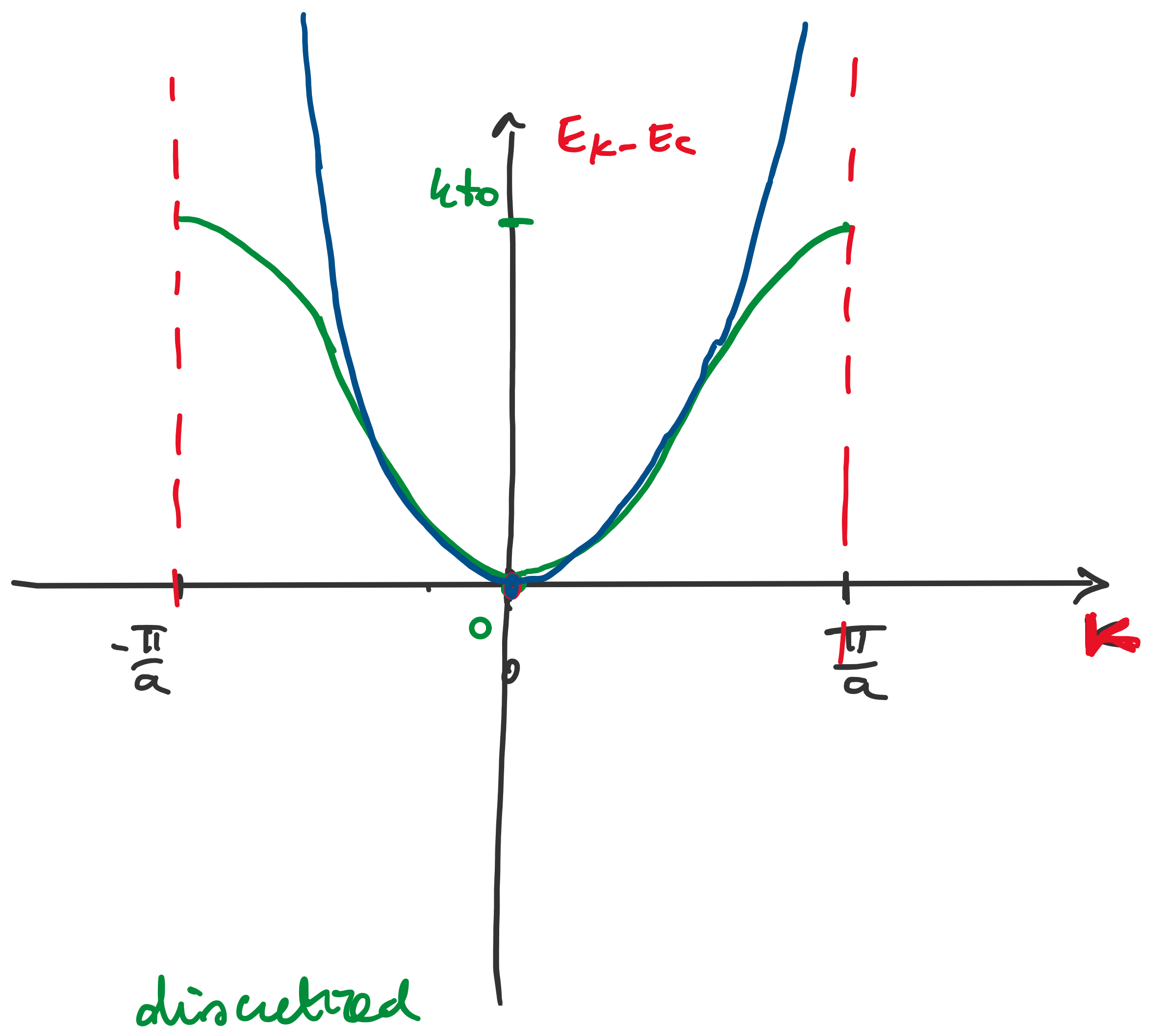
If I divide by e^{jkna}

$$-t_0\left[e^{jka} - 2 + e^{-jka}\right] = (\overset{E_k}{E} - E_c)$$

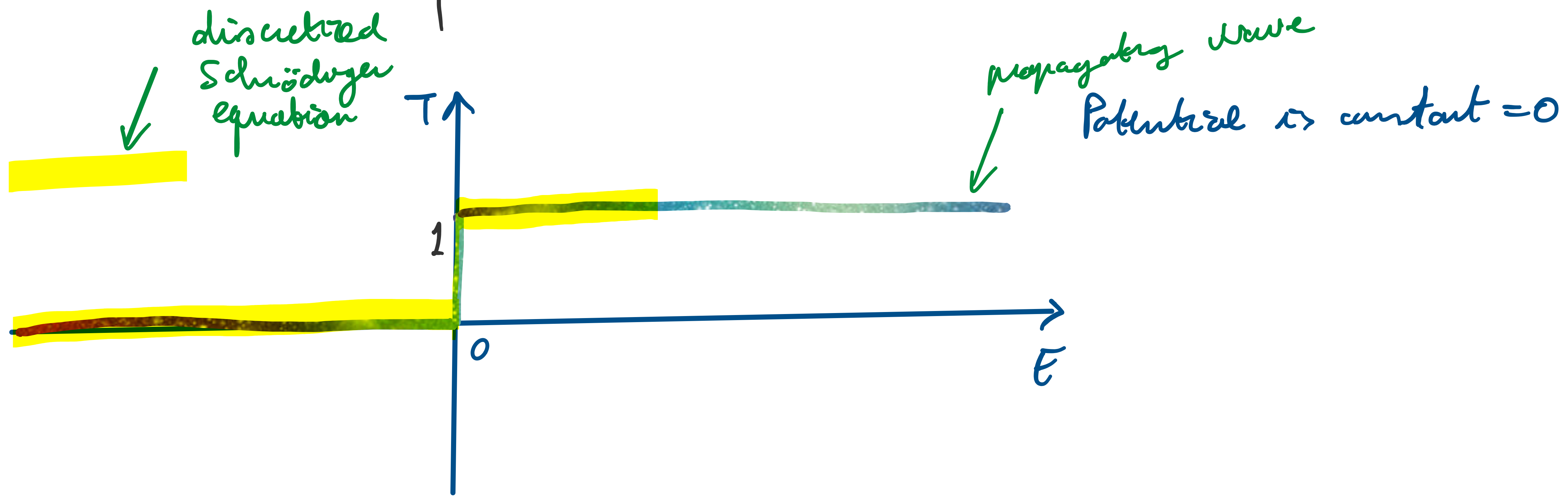
$$\boxed{E_k = E_c - t_0\left[2\cos ka - 2\right] = E_c + 2t_0\left[1 - \cos ka\right]}$$

$ka \ll 1$ $\quad 1 - \cos ka \simeq 1 - \left[1 - \frac{k^2a^2}{2}\right] \simeq \frac{k^2a^2}{2}$

$ka \ll 1$ $\quad E_k \simeq E_c + \frac{\hbar^2k^2}{2m^*}$



The dispersion relation can be approximated to a parabola if $E_k - E_c \ll 4t_0$



Exercise on python