

$$\Psi_x(L, t) = - \sqrt{\frac{2}{\hbar\pi}} e^{-i\frac{\pi}{4}} e^{-i\frac{V_L}{\hbar}t} \frac{d}{dt} \int_0^t \frac{\Psi(L, \tau)}{\sqrt{t-\tau}} e^{+i\frac{V_L}{\hbar}t} d\tau.$$

In contrast with *Dirichlet conditions*, they are not stagnant in time and the numerical method requires the storage of the past history values at all time levels at the boundaries. The convolution term on the right hand side of the equation (38) appears as a fractional $(\frac{1}{2})$ time derivative. Derivation of the *DTBCs* uses the *Crank-Nicholson scheme* at a discrete level. The discrete *TBCs* for the one dimensional Schrödinger equation for $n \geq 1$ on the right is at $j = J$

$$\Psi_{J-1}^n - l_J^n \Psi_J^n = \sum_{k=1}^{n-1} l_J^{(n-k)} \Psi_J^k - \Psi_{J-1}^{n-1} \quad (38)$$

with,

$$\begin{aligned} l_j^n &= \left(1 - i\frac{R}{2} + \frac{\sigma_j}{2}\right) \delta_n^0 + \left(1 + i\frac{R}{2} + \frac{\sigma_j}{2}\right) \delta_n^1 + \alpha_j e^{-in\varphi_j} \frac{P_n(\mu_j) - P_{n-2}(\mu_j)}{2n-1}, \\ R &= \frac{4}{\hbar} \frac{(\Delta x)^2}{\Delta t}, \quad \varphi_j = \arctan \frac{2R(\sigma_j+2)}{R^2-4\sigma_j-\sigma_j^2}, \\ \mu_j &= \frac{R^2+4\sigma_j+\sigma_j^2}{\sqrt{(R^2+\sigma_j^2)(R^2+[\sigma_j+4]^2)}}, \quad \sigma_j = 2(\Delta x)^2 V_j, \\ \alpha_j &= \frac{i}{2} \sqrt[4]{(R^2+\sigma_j^2)(R^2+[\sigma_j+4]^2)} e^{i\frac{\varphi_j}{2}}. \end{aligned}$$

The Right discrete boundary condition is derived at $i = imax - 1$

$$- \Psi_{imax}^n + \mathbb{C} \Psi_{imax-1}^n - \Psi_{imax-2}^n = \quad (39)$$

$$\Psi_{imax}^{n-1} - \mathbb{C}' \Psi_{imax-1}^{n-1} + \Psi_{imax-2}^{n-1} = b^{n-1} (imax - 1) \quad (40)$$

where

$$i = L, \Psi_{imax}^n = \Psi(L, t), \quad (41)$$

the *Right Transparent Boundary Condition*, is part of the system of equations. The *Discrete Transparent Boundary Condition* (38) is:

$$\begin{aligned} \Psi_{imax-1}^{n+1} - l_{imax}^{(0)} \Psi_{imax}^{n+1} &= \\ \sum_{k=1}^{n-1} l_{imax}^{(n-k)} \Psi_{imax}^k - \Psi_{imax-1}^n &= b^{n-1} (imax). \end{aligned} \quad (42)$$

Note that $b^{n-1}(imax)$ will change at every time level n . This is the value at that boundary