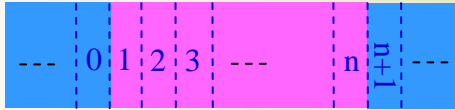


Improved transfer matrix method without numerical instability

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What's transfer matrix (TMM) ?



$$\Phi(n+1) = T_{n+1} T_C^n T_0 \Phi(0) \quad (1)$$

TMM transfer wave function from one site to another. TMM is widely used in: Electronic Transport; Photonics; Electromagnetics; Acoustics; Seismology. But the numerical instability seriously limit its further application!

New improved TMM

Our method is to eliminate the divergence originating term $\exp(-ik_j n x + \theta n x)$. Induce new variables $\{v_p\}$

$$\begin{pmatrix} \vdots \\ \{v_j\} \end{pmatrix} e^{ik_j x - \theta x} = \widetilde{T}_0 \begin{pmatrix} \{t\} \\ 0 \end{pmatrix} \quad (4a)$$

$$\begin{pmatrix} In \\ \{r\} \end{pmatrix} = \widetilde{T}_{n+1} \begin{pmatrix} \vdots \\ \{v_j\} \end{pmatrix} \quad (4b)$$

From eq. (4a), (4b), we get an expanded equation set

$$A' \begin{Bmatrix} \{t_i\} \\ \{v_j\} \end{Bmatrix} = b' \quad (5)$$

The elements of matrix A' are finite now. $\{t_i\}, \{r_i\}$ can be got without numerical instability.

Numerical Instability of TMM

Transform eq.(1) to k-space:

$$\psi(n+1) = \widetilde{T}_{n+1} \widetilde{T}_C^n \widetilde{T}_0 \psi(0)$$

$$\begin{pmatrix} In \\ \{r\} \end{pmatrix} = \widetilde{T}_{n+1} \begin{pmatrix} \{e^{ik_j x}\} & 0 & 0 & 0 \\ 0 & \{e^{ik_j x - \theta x}\} & 0 & 0 \\ 0 & 0 & \{e^{-ik_j x}\} & 0 \\ 0 & 0 & 0 & \{e^{-ik_j x + \theta x}\} \end{pmatrix} \widetilde{T}_0 \begin{pmatrix} \{t\} \\ 0 \end{pmatrix} \quad (2)$$

$$\left| \{e^{ik_j x}\} \right| = 1; \left| \{e^{ik_j x - \theta x}\} \right| < 1; \left| \{e^{-ik_j x}\} \right| = 1; \left| \{e^{-ik_j x + \theta x}\} \right| > 1.$$

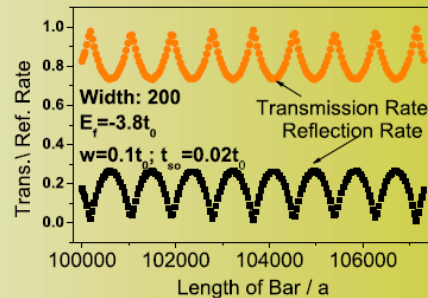
Reconstruct eq.(2) to get eq.(3) to solve $\{t\}$ and $\{r\}$.

$$A\{t\} = b; \{t\} = A^{-1}b \quad (3)$$

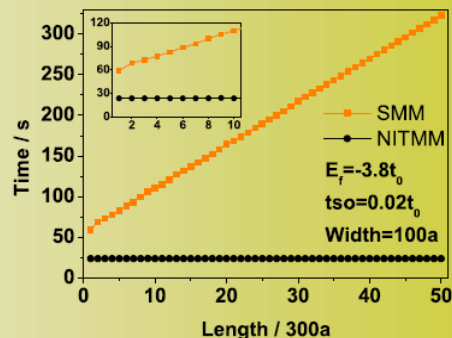
when the transfer step number n is large, the inverse of matrix A will meet the problem of numerical overflow due to the term: $\exp(-ik_j n x + \theta n x)$.

Examples of Application

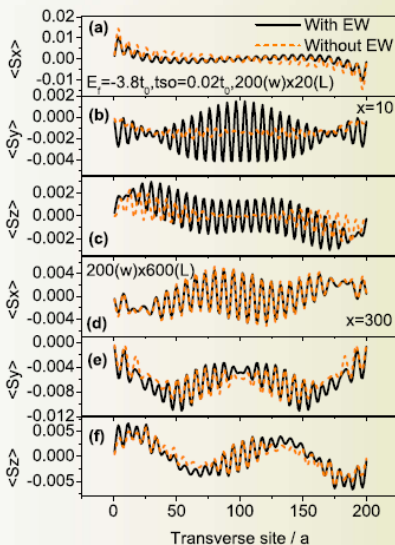
I. Capability to deal with extreme long length.



II. The computing time is the zeroth order of length.



III. The effect of evanescent wave is considered exactly.



Reference:

HuiQiong Yin and Ruibao Tao, EPL 84(2008), 57006. And all the references therein.