Non-Equilibrium Electron Transport using DMRG

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- The time evolution operator.
- DMRG procedure.
- Wave packet dynamics.
- A tribute to discussions: the ground state curvature
- Interacting System with Leads.
- Imaginary time dynamics.
- Finite bias conductance.
- Summary.

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Real-Time Dynamics:
The Time Evolution Operator

The time evolution operator

$$\hat{U}(t,t') = \mathcal{T}\,\mathrm{e}^{\int_{t'}^{t} \imath\mathcal{H}(t'')\mathrm{d}t''}$$

contains the complete dynamics of the system.

For time independent Hamilton operators one gets

$$\hat{U}(t',t) = \mathrm{e}^{\imath\mathcal{H}(t'-t)} \qquad |\Psi(t')\rangle = \mathrm{e}^{\imath\mathcal{H}(t'-t)}|\Psi(t)\rangle$$

Improving convergence:

$$\begin{aligned} \hat{P} &= \sum_{m=0}^{m-1} |\Psi_m\rangle\langle\Psi_m| \\ |\xi(t)\rangle &= \sum_{m=0}^{m-1} \mathrm{e}^{-\imath(E_m-E_0)t}|\Psi_m\rangle\langle\Psi_m \mid \xi(0)\rangle \\ &\quad + \mathrm{e}^{-\imath(\mathcal{H}-E_0)t}(1-\hat{P})|\xi(0)\rangle\,, \end{aligned}$$

The Matrix Exponential $\mathrm{e}^{\imath\mathcal{H}t}x$

Arnoldi type iterative Krylov space method:

- Start iteration with $\ell = 5$.
- Calculate a basis $\{b_j\}$, $b_1 = x/||x||$, of the Krylov space $K_x^\ell(\mathcal{H}) = \mathrm{span}\{x, \mathcal{H}x, \mathcal{H}^2x, \cdots, \mathcal{H}^{\ell-1}x\}$.
- Calculate the projection $\mathcal{H}|_K^\ell$ of $\mathcal{H}$ on $K_x^\ell(\mathcal{H})$.
- Calculate the full matrix exponential $E^\ell = e^{\imath t\mathcal{H}|_K^\ell}$.
- Iterate until $r = \sum_{j=\ell-2}^{\ell} |E_{j,1}^\ell|$ is below a desired threshold, e.g. 10^{-9}.
- Finally: $\mathrm{e}^{-\imath\mathcal{H}t}x = ||x|| \sum_{j=1}^{\ell} E_{j,1}^\ell b_j$.

The Matrix Exponential $\mathrm{e}^{\imath\mathcal{H}t}x$

Remarks:

- $\mathcal{H}|_K^\ell$ is directly given by the orthogonalization of the basis.
- Arnoldis method gives an $\ell \times (\ell + 1)$ matrix $\mathcal{H}|_K^\ell$.
- Hermitian $\mathcal{H}$ lead to a tridiagonal $\mathcal{H}|_K^\ell$.
- Method works also for non-hermitian matrices $\mathcal{H}$.
- Can be easily adapted to arbitrary matrix function.

DMRG procedure for $|\xi(T)\rangle = \mathrm{e}^{-\imath\mathcal{H}T}|\xi(0)\rangle$

- Warm up: Infinite lattice sweep with $|\Psi_m\rangle$, $|\xi(0)\rangle$ and $|\Psi_0^0\rangle$.
- Standard finite lattice sweep DMRG procedure.
  - Calculate initial state $|\xi(0)\rangle$
  - Discretize the time interval into N_T time steps: $\{t_0, t_1, t_2, \cdots, t_N\}$ with $t_0 = 0$, $t_j < t_{j+1}$ and $t_N = T$.
  - $|\xi(t_j)\rangle = \mathrm{e}^{-\imath\mathcal{H}(t_j - t_{j-1})}|\xi(t_{j-1})\rangle$
  - $\rho = \mathrm{Tr}\left(\sum_m |\Psi_m\rangle\langle\Psi_m| + \sum_{j=0}^{N} |\xi(t_j)\rangle\langle\xi(t_j)|\right)$.
- Implicit combining of operators.
- Keeping the dimension of the superblock fixed during a sweep.
- Calculate density in the last 1.5 sweeps.
- Parallelized scalar product, overlapping scheduling for $\mathrm{e}^{-\imath\mathcal{H}t}$.
- Note: Ψ_m are not needed.

The Model:
Interacting System with Leads

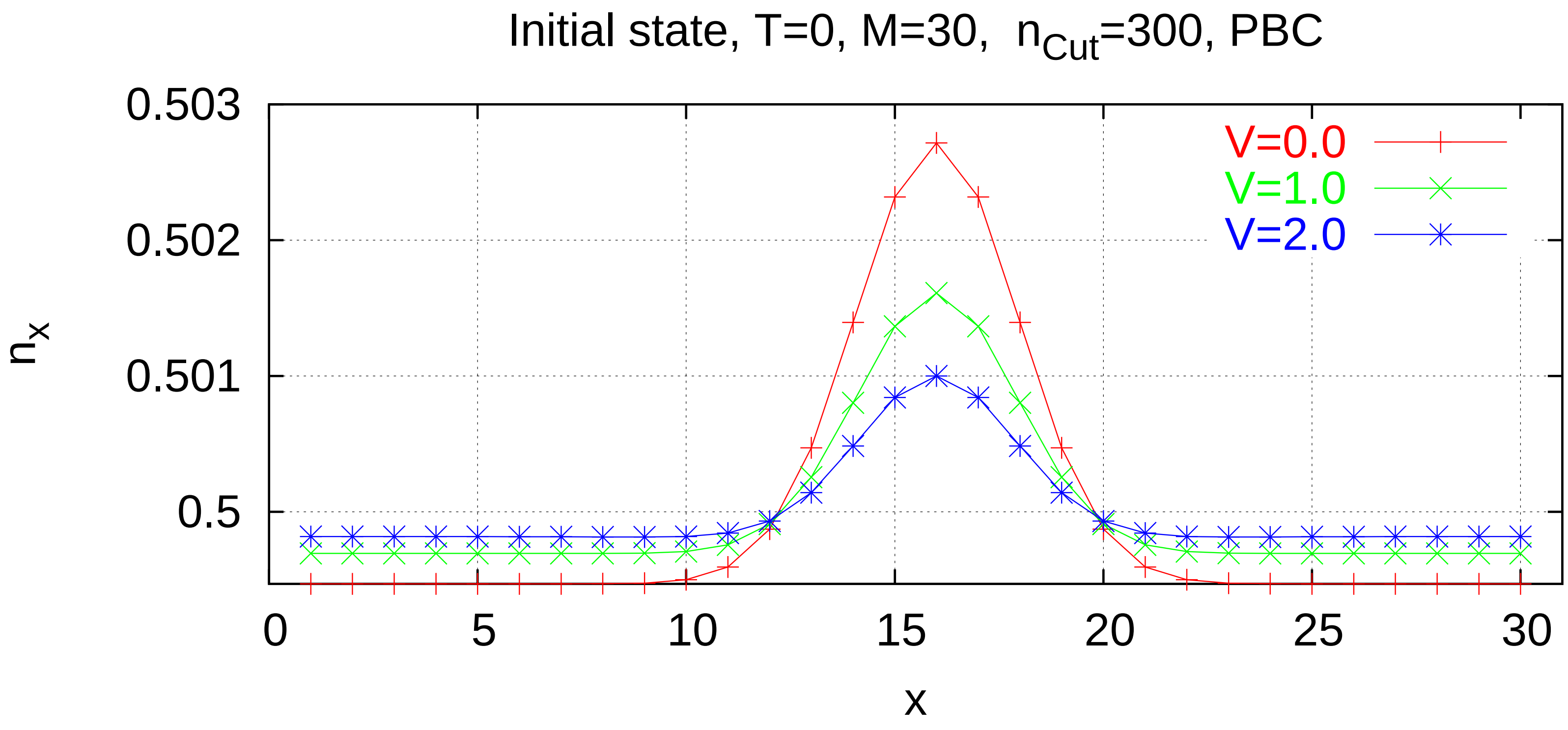
$$\mathcal{H} = \underbrace{-\sum_{l=\ell}^{M} t_\ell \, c_\ell^\dagger c_{\ell-1} \; + \; t_\ell^* \, c_{\ell-1}^\dagger c_\ell}_{\text{Kinetic energy}} + \underbrace{\sum_{\ell=1}^{M} \mu_\ell \, n_\ell}_{\text{On}-\text{site potential}} + \underbrace{\sum_{s=1}^{\bar{s}} \sum_{\ell=1}^{M} U_{s,\ell} \, n_\ell n_{\ell-s}}_{\text{Interaction}}$$

- Number of sites: $M = M_L + M_S$.
- Number of fermions: $N = \sum_{l=1}^{M} n_l = \sum_{l=1}^{M} c_l^\dagger c_l$.
- Filling $\rho = N/M$.
- Range of the interaction: $\bar{s}$.

Homogenous System, PBC

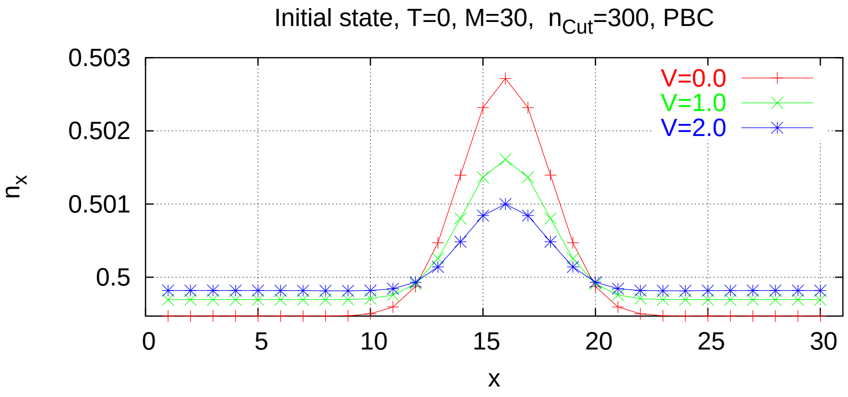
Initial state:

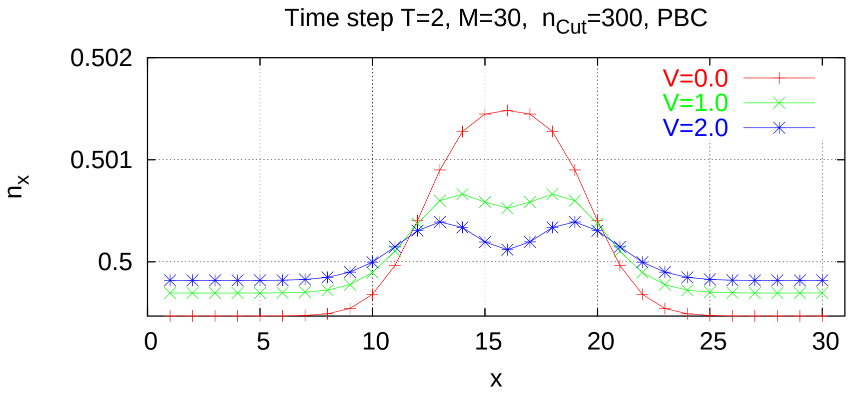
$$\begin{aligned} \mathcal{H}' &= \mathcal{H} + \delta\mathcal{H} \\ \delta\mathcal{H} &= -\mu \sum_{x=1}^{M} \mathrm{e}^{-\frac{(x-x_1)^2}{2\sigma^2}} n_x \end{aligned}$$

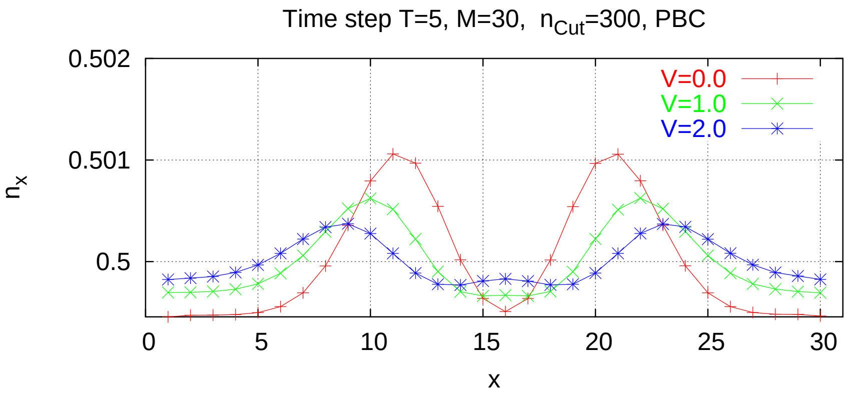


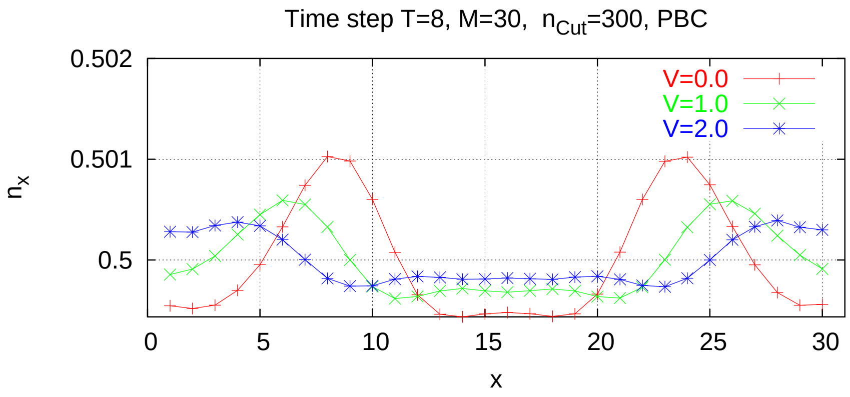
Homogenous System, PBC

$M_L = 30$, $M_S = 0$, $N = 15$, periodic boundary conditions.


Initial state, T=0, M=30, n_{Cut}=300, PBC


Time step T=2, M=30, n_{Cut}=300, PBC


Time step T=5, M=30, n_{Cut}=300, PBC


Time step T=8, M=30, n_{Cut}=300, PBC

Homogenous System, PBC

$M_L = 30$, $M_S = 0$, $N = 15$, periodic boundary conditions.

V	-1.5	0.0	0.5	1.0	1.5
v_g, $\mu = 0.02$	1.0	1.9	2.2	2.47	2.71
v_g, $\mu = 0.002$	0.92	2.00	2.30	2.59	2.87
v_F(BA)	0.88	2.00	2.31	2.60	2.88

Comparison of v_g extracted from DMRG simulations for a $M = 30$ site system and a potential strength $\mu = 0.02$, $\mu = 0.002$ and Bethe ansatz results for v_F in the infinite system and an infinitesimal small excitation.

Conformal field theory:

$$\begin{aligned} C &= M \left. \frac{\partial^2 E_0(\phi)}{\partial \phi^2} \right|_{\phi=0} = v_c K/\pi \\ E_0(M)/M &= e(\infty) - \frac{\pi}{6M^2} v_c \end{aligned}$$

The ground state curvature $C = M \left.\frac{\partial^2 E_0(\phi)}{\partial \phi^2}\right|_{\phi=0}$ can be obtained for a non-degenerate ground state from

$$
\begin{aligned}
E^{(1)} &= \langle \Psi^{(0)} |\, \imath \hat{J} \,| \Psi^{(0)} \rangle = 0 \\
E^{(2)} &= \langle \Psi^{(0)} |\, \hat{T} \,| \Psi^{(0)} \rangle \; + \; 2 \langle \Psi^{(0)} |\, \imath \hat{J} \,| \Psi^{(1)} \rangle \,,
\end{aligned}
$$

where $|\Psi^{(1)}\rangle$ is given by solving the linear set of equations

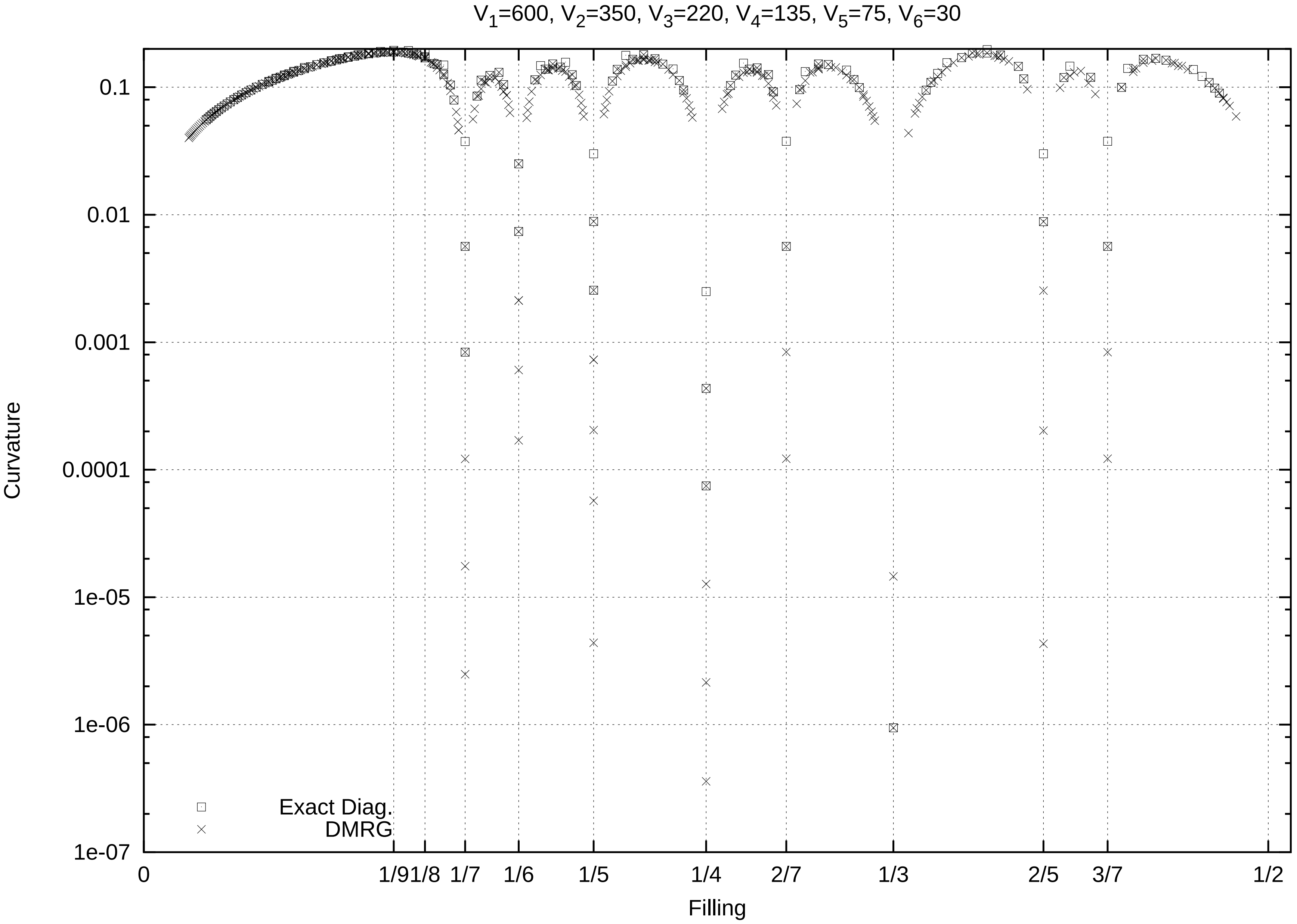
$$\left(\mathcal{H}^{(0)} - E^{(0)} \right) | \Psi^{(1)} \rangle = - \imath \hat{J} \,| \Psi^{(0)} \rangle$$

on the subspace orthogonal to the ground state.

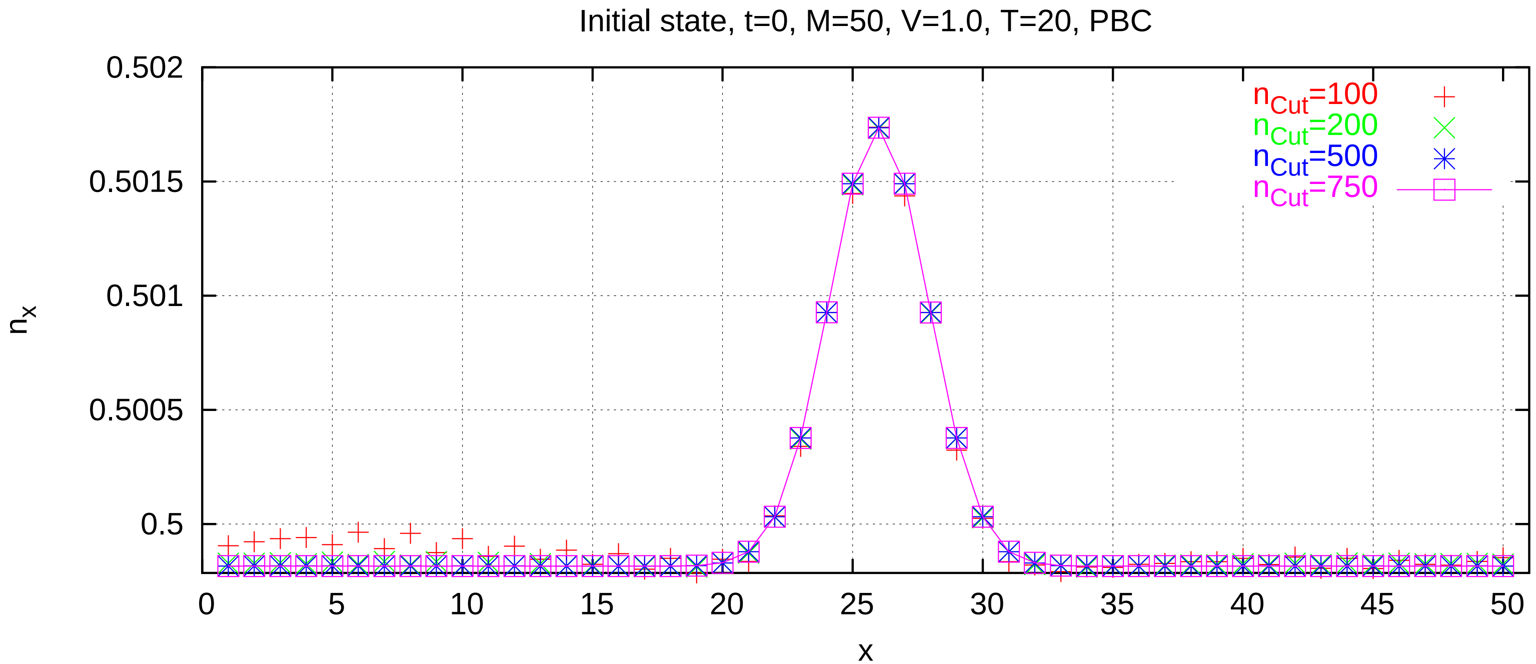
Remarks:

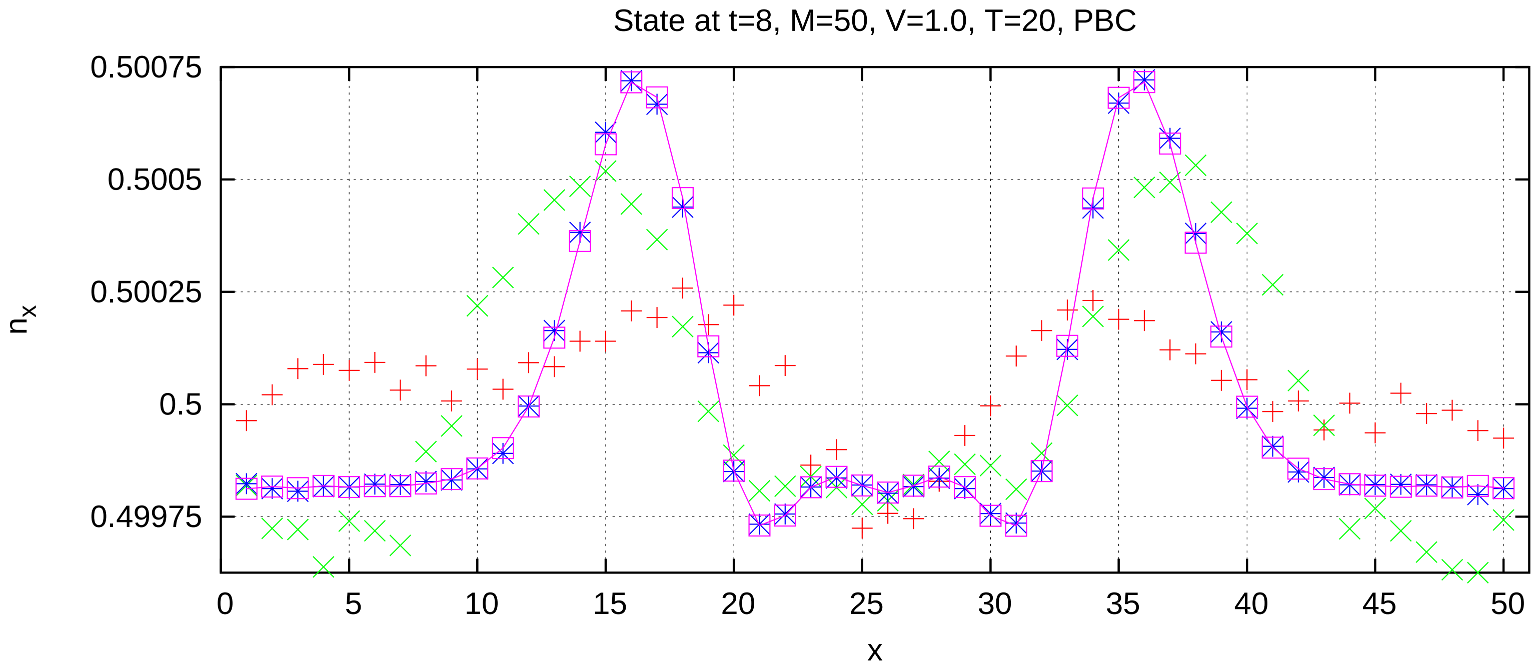
- Only ground state, $\mathcal{H}$, $\hat{T}$ and $\hat{J}$ is needed.
- $|\Psi^{(1)}\rangle$ is purely imaginary.
- $|\xi\rangle = \imath |\Psi^{(1)}\rangle$ leads to real equations.
- $C = M E^{(2)}$ is evaluated at strictly $\phi = 0$ (important for commensurability effects).
- This method is just standard perturbation theory in a non-diagonal basis.
- Extension to degenerate ground states and higher order derivatives is straightforward, similar to Brillouin-Wigner perturbation theory.

Multiple Umklapp Scattering:

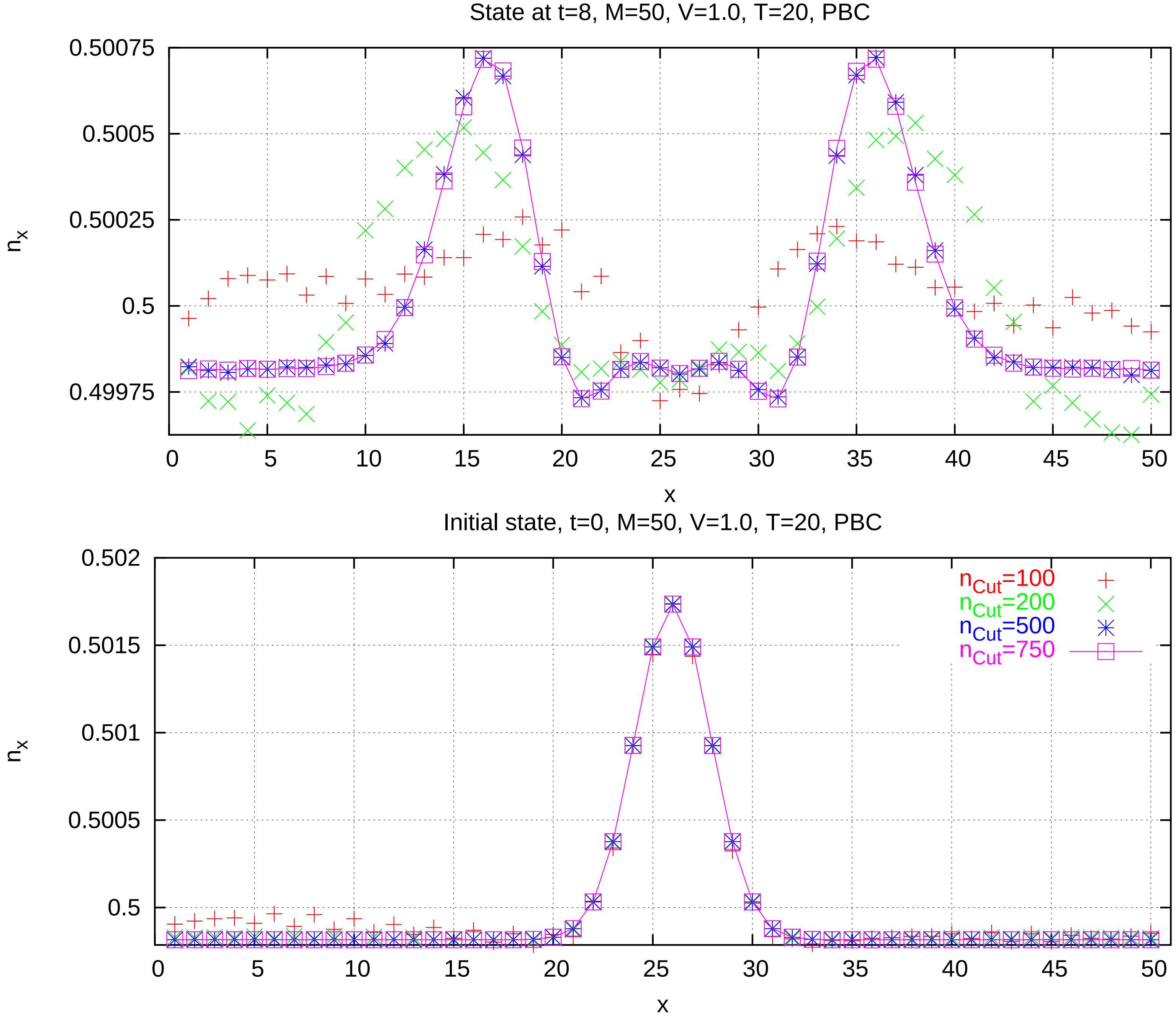


Accuracy?

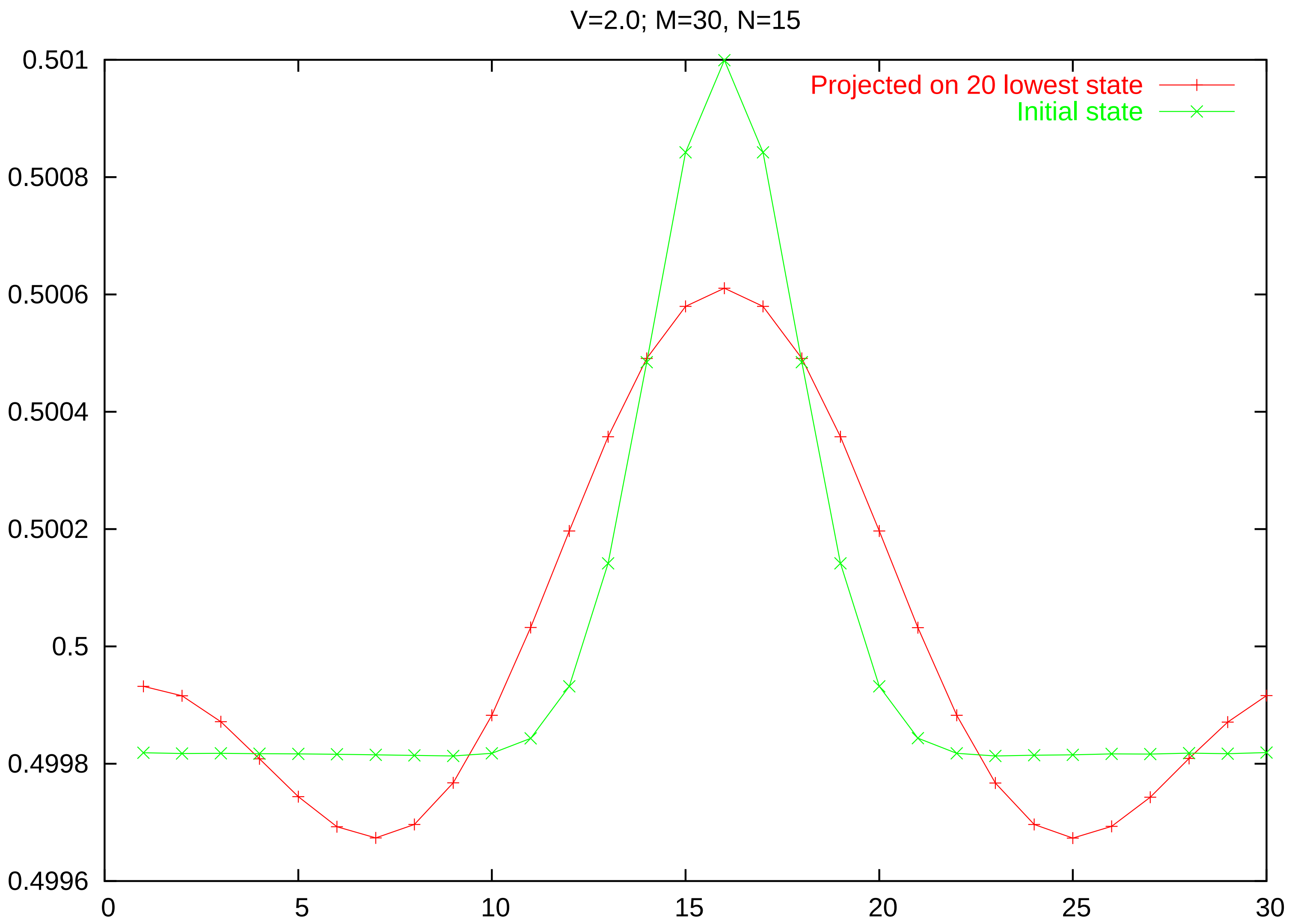

Initial state, t=0, M=50, V=1.0, T=20, PBC


State at t=8, M=50, V=1.0, T=20, PBC

Accuracy?


State at t=8, M=50, V=1.0, T=20, PBC
0.50075
0.5005
0.50025
0.5
0.49975
n_x
0
5
10
15
20
25
30
35
40
45
50
x
Initial state, t=0, M=50, V=1.0, T=20, PBC
0.502
0.5015
0.501
0.5005
0.5
n_x
x
n_{Cut}=100
n_{Cut}=200
n_{Cut}=500
n_{Cut}=750

Projection on low energy subspace



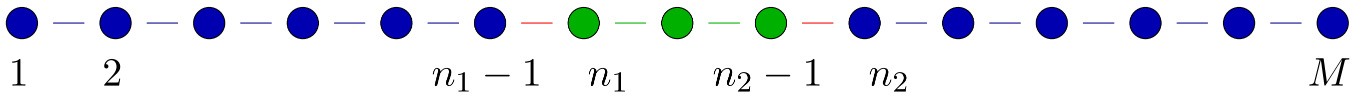
Interacting Nano-System

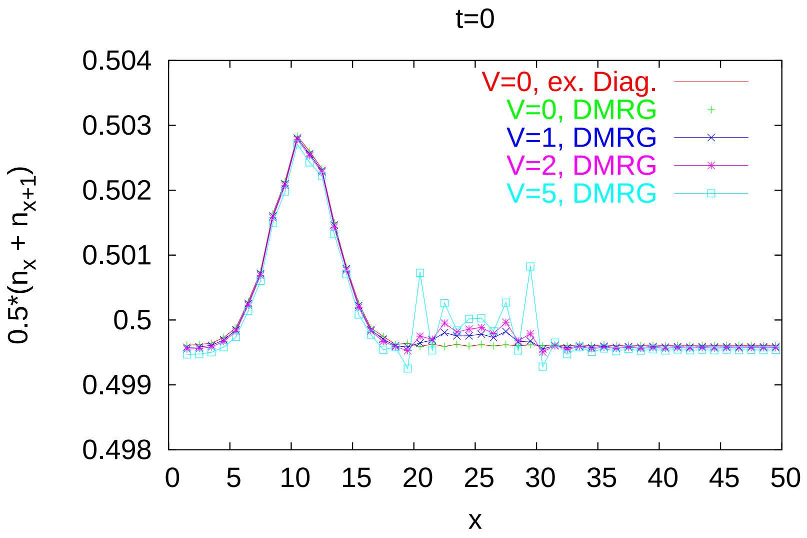
$M_L = 43,\ M_S = 7,\ N = 25,\ t' = 1.0$, hard wall BC, $n_{\mathrm{Cut}} = 1000$.

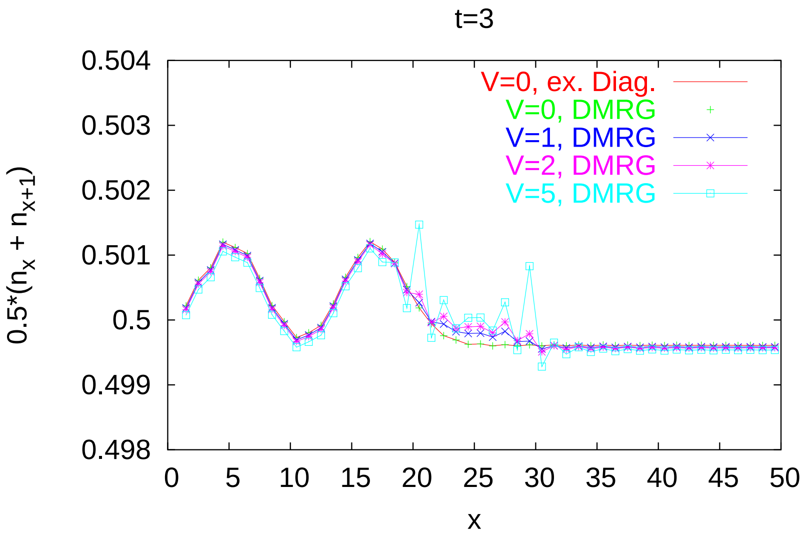
Left Lead
$M_L/2$ sites

Nano System
M_S sites

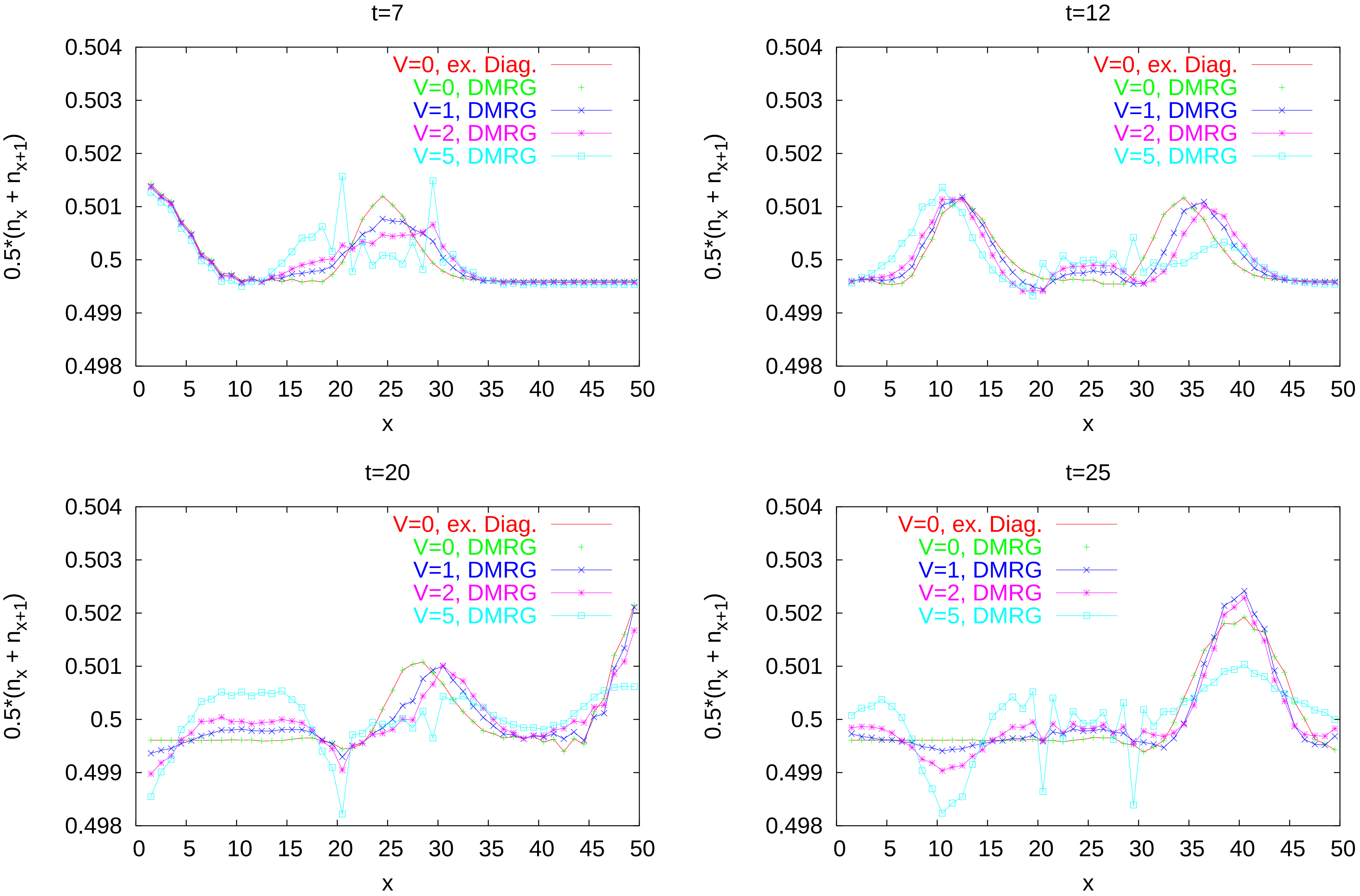
Right Lead
$M_L/2$ sites





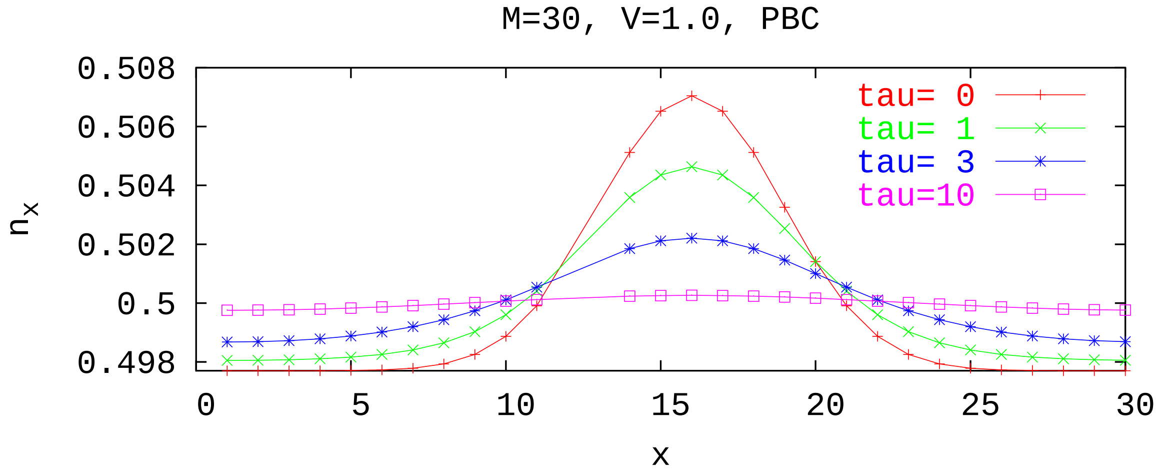


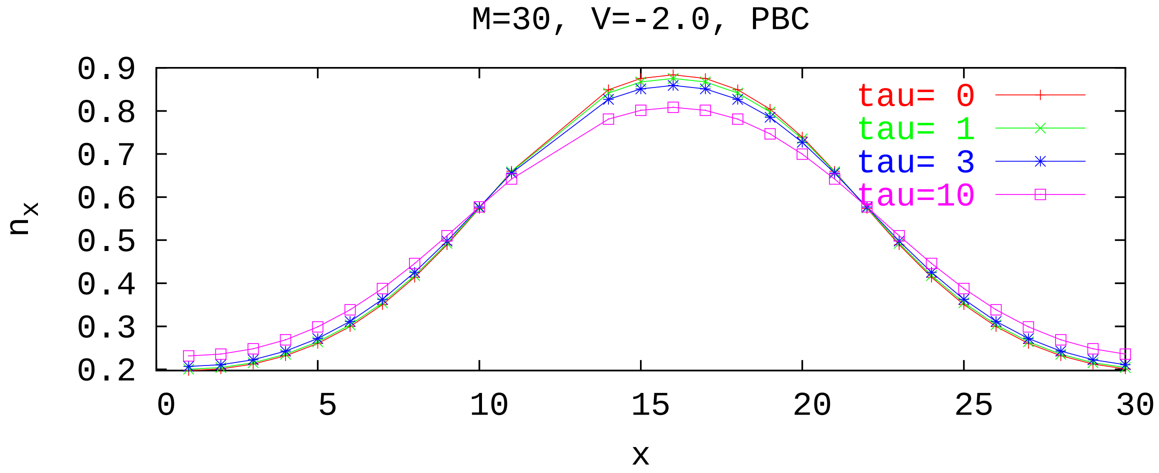
Interacting Nano-System, $M_L = 43$, $M_S = 7$, $N = 25$, $t' = 1.0$



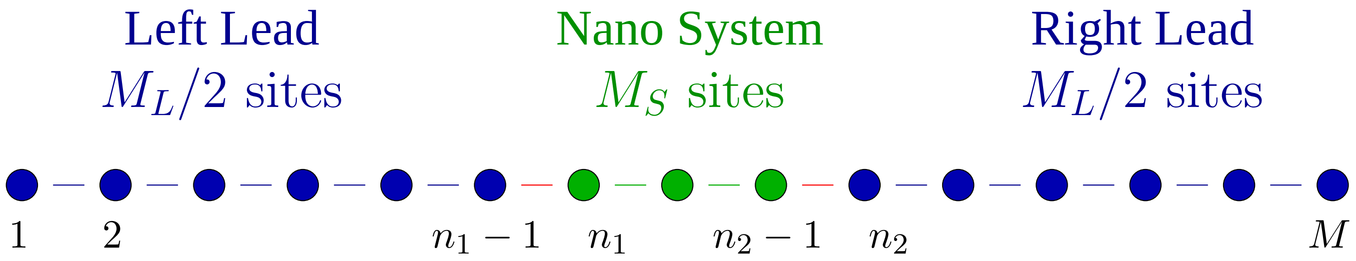
Imaginary time dynamics: $\hat{U}(\tau) = \mathrm{e}^{-\mathcal{H}\tau}$

$M_L = 30$, $M_S = 0$, $N = 15$, periodic boundary conditions.


M=30, V=1.0, PBC


M=30, V=-2.0, PBC

Conductance of a nano structure coupled to leads



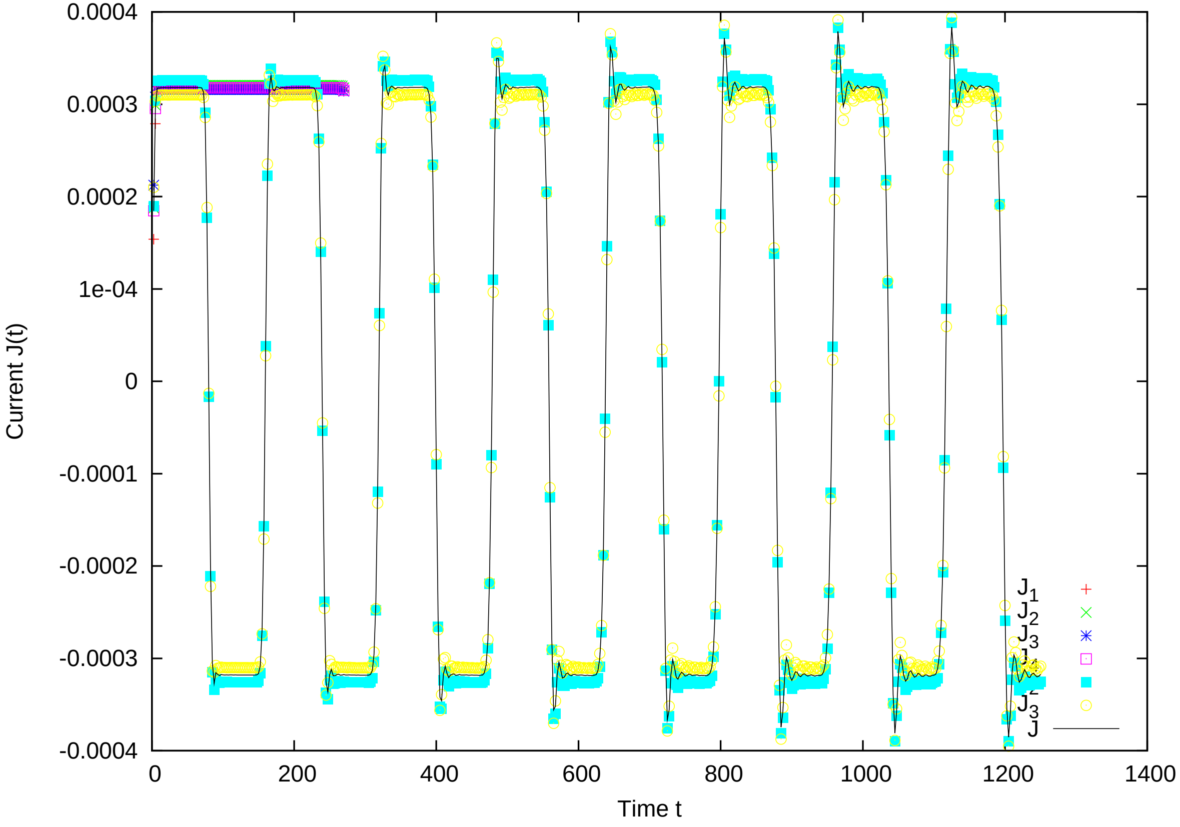
Left Lead
$M_L/2$ sites

Nano System
M_S sites

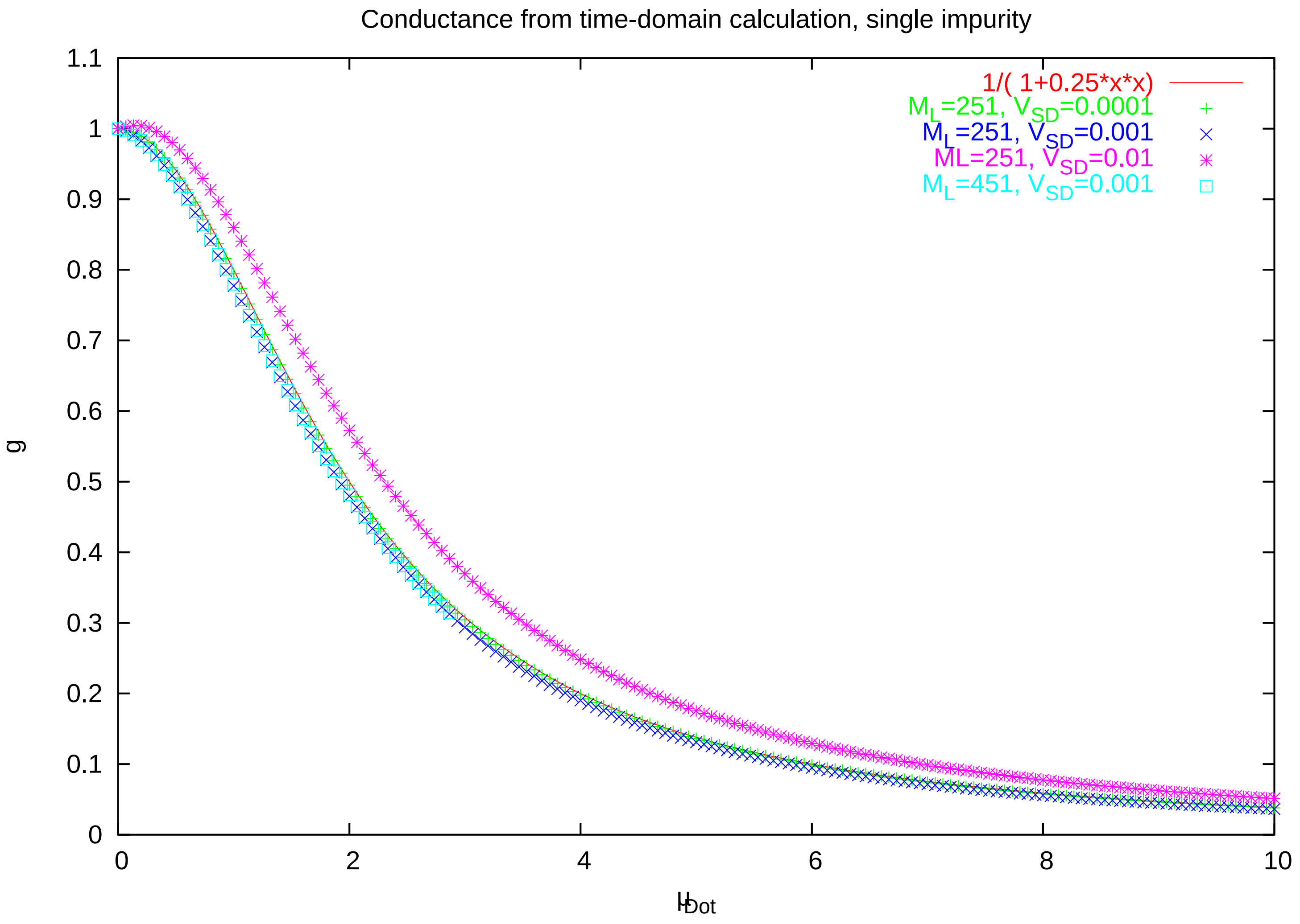
Right Lead
$M_L/2$ sites

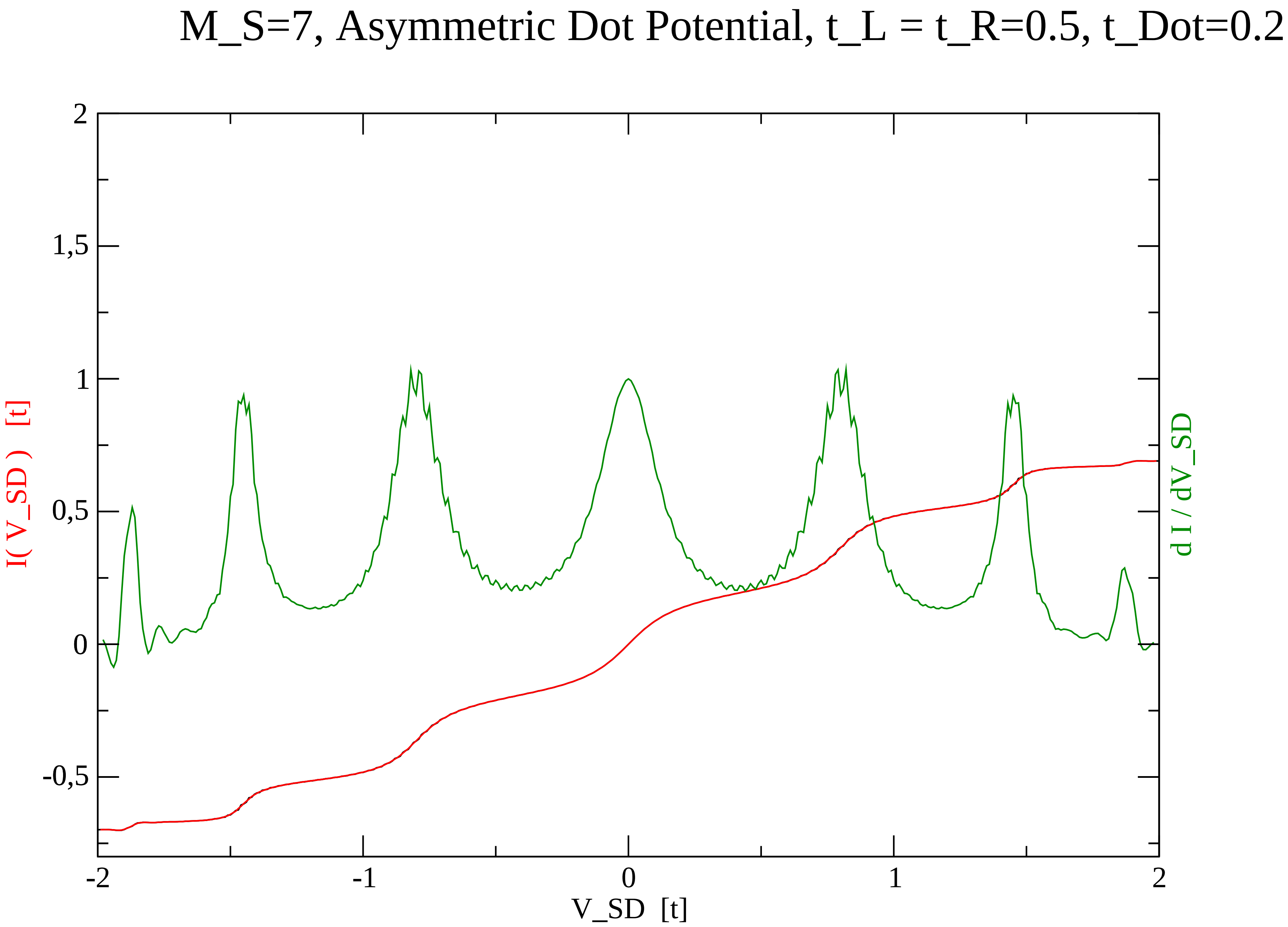
- Start with an excitation extented over the complete leads.
- Perform the time evolution.
- Measure the current J close to the nano structure.
- Look for a quasi-stationary state.
- Calculate $g = J/\mu_{SD}$.

Quasi-stationary state



Zero bias conductance: resonant tunneling




M_S=7, Asymmetric Dot Potential, t_L = t_R=0.5, t_Dot=0.2
I(V_SD) [t]
d I / dV_SD
V_SD [t]
2
1,5
1
0,5
0
-0,5
-2
-1
0
1
2

Summary

- Time evolution using the matrix exponential within an quasi-exact DMRG.
- Simple way of of constructing initial wave packets.
- Direct calculation of the excitation velocity.
- Need for high-energy states.
- Finite bias conductance.

Outlook

- Optimize parallelization.
- Apply ideas from DMRG'04 workshop.
- Design of electronic devices.