Methods for Real time Dynamics

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Contents:

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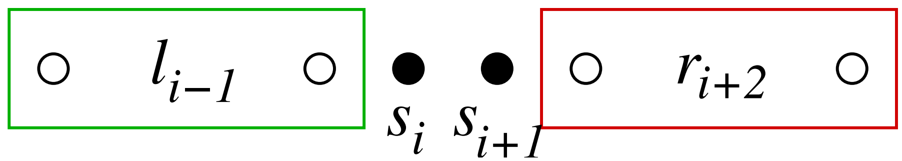
Wavefunction Transformations

Original usage: Transform wavefunction from one step to the next as a guess for Lanczos/Davidson— for optimization only.

Now essential for real-time algorithms.



$$|\psi\rangle = \sum_{l_{i-1},s_i,s_{i+1},r_{i+2}} \psi(l_{i-1}, s_i, s_{i+1}, r_{i+2}) |l_{i-1} s_i s_{i+1} r_{i+2}\rangle$$

Density matrix: $\rho_{l_{i-1},s_i;l'_{i-1},s'_i}$

Its eigenvectors: $\xi^{\alpha}_{l_{i-1},s_i}$ New basis: $|\alpha\rangle = \sum_{l_{i-1},s_i} \xi^{\alpha}_{l_{i-1},s_i} |l_{i-1} s_i\rangle$

Wavefunction in new basis:

$$|\psi'\rangle = \sum_{\alpha=1}^{m} \sum_{s_{i+1},r_{i+2}} \psi(\alpha, s_{i+1}, r_{i+2}) |\alpha s_{i+1} r_{i+2}\rangle$$

with

$$\psi(\alpha, s_{i+1}, r_{i+2}) = \sum_{l_{i-1}, s_i} \xi^{\alpha}_{l_{i-1}, s_i} \psi(l_{i-1}, s_i, s_{i+1}, r_{i+2})$$

Error in transformation: can show $\langle \psi' | \psi \rangle = 1 - \text{truncation \ error}$

Matrix product notation: relabel $\alpha \to l_i$ and define $A^i[s_i]_{l_{i-1}, l_i} = \xi^{l_i}_{l_{i-1}, s_i}$. Then

$$|l_i\rangle = \sum_{l_{i-1}, s_i} A^i[s_i]_{l_{i-1}, l_i} |l_{i-1} s_i\rangle$$

The right block came from a similar process:

$$|r_{i+2}\rangle = \sum_{s_{i+2}, r_{i+3}} B^{i+2}[s_{i+2}]_{r_{i+2}, r_{i+3}} |s_{i+2} r_{i+3}\rangle$$

This is exact: the error came in the previous sweep when r_{i+2} was generated. This gives the wavefunction in the basis of the next step:

$$\psi(l_i, s_{i+1}, s_{i+2}, r_{i+3}) = \sum_{l_{i-1}, s_i, r_{i+2}} A^i[s_i]_{l_{i-1}, l_i} \psi(l_{i-1}, s_i, s_{i+1}, r_{i+2}) B^{i+2}[s_{i+2}]_{r_{i+2}, r_{i+3}}$$

We can write the wavefunction without any sites in the center:

$$|\psi\rangle = \sum_{l_i, r_{i+1}} \psi(l_i, r_{i+1}) |l_i r_{i+1}\rangle$$

On the other hand, if we expand out using the A and B matrices out to the end, we get the matrix product expression [Ostlund and Rommer, PRL 75, 3537 (1995)]:

$$|\psi\rangle = \sum_{s_1 \ldots s_N} A^1[s_1] \ldots A^i[s_i] \psi B^{i+1}[s_{i+1}] \ldots B^N[s_N] |s_1 \ldots s_N\rangle$$

Here the first A and last B are vectors. If we are targetting several states ψ_t the only change is to the central ψ matrix. We can move the dividing line all the way to the right or left to get only A's or B's. We can also write it as a trace, which allows one to use periodic BCs. The representation for PBCs is compact, but obtaining it requires CPU time of order m^5 (re: Verstraete's talk) instead of the usual m^3.

Targetting and Operators

Our DMRG basis is only guaranteed to represent targetted states, and those only after enough sweeps!

$$\rho = \sum_t w_t \psi^t \psi^{tT}$$

We can obtain exact operator expectation values $\langle \psi^{t'} | O | \psi^t \rangle$ if we have generated matrix elements $O_{\alpha\alpha'}$ correctly: if

$$O = \sum_\beta A_i^\beta B_j^\beta C_k^\beta \ldots, \qquad i, j, k \; sites$$

we generate each term β separately, then add. Call this "site expansion".

If $O = PQ$, we have two choices:

- 1) generate the site expansion for O (typically N^2 terms).
- 2) Calculate $|\phi\rangle = Q|\psi^t\rangle$, target it, and sweep to make the basis represent it. Then

$$\langle \psi^{t'} | O | \psi^t \rangle = \langle \psi^{t'} | P | \phi \rangle$$

2) requires a larger basis but is usually faster, and can be easily generalized to bigger products. 2) is used in freq. dynamics. One should keep in mind that 1) is always a possibility.

I propose the terms “quasiexact” and/or “controlled by the truncation error” to mean approximate algorithms whose errors are strictly controlled by the truncation error ϵ (normally proportional to ϵ or $\epsilon^{1/2}$). The infinite system method applied to a finite system is not quasiexact, even though the error goes to zero as $m \to \infty$.

Non quasiexact algorithms seem to be the source of almost all DMRG “mistakes”.

Real time dynamics

Previous approaches

- Cazalilla and Marston, PRL 88, 256403 (2002). They used the infinite system method to find the ground state, and evolved in this fixed basis by solving the Schrödinger equation, w/o sweeps. They applied it to fermion chains under an applied field. This is not quasiexact, and one expects it to fail, but they found it worked OK for short to moderate times, in the models considered.

- Luo, Xiang, and Wang (LXW), PRL 91, 049701 (2003), showed how to target correctly for real time dynamics. Their method is quasiexact if you add sweeping. They target

  $$\psi(t=0), \psi(t=\Delta), \psi(t=2\Delta), \psi(t=3\Delta), \mathrm{etc.}$$

  With sweeping, this is quasiexact as $\Delta \to 0$, and one expects rapid convergence with Δ. One can integrate the Schrödinger equation in a variety of ways, for example, using Runge-Kutta.

LXW's method is slow, and if you add sweeping to make it quasiexact, it is very very slow. One does the whole time evolution at each DMRG step! It also targets many states, so a large m is needed.

Vidal's Trotter approach

Guifre Vidal, whose background is quantum information, reinvented part of DMRG and came up with a very efficient time evolution method, based on the matrix product representation. Later, Feiguin and I, and separately Daley, Kollath, Schollwoeck, and Vidal showed how to translate the ideas to DMRG, where it is easier for us to understand:

The key new idea: the second order Suzuki-Trotter decomposition for a short time τ is

$$e^{-i\tau H} \approx e^{-i\tau H_A/2} e^{-i\tau H_B} e^{-i\tau H_A/2},$$

where $H = H_A + H_B$. Here we make A the even bonds and B the odd, 1D only. The individual link-terms $\exp(-i\tau H_j)$ (coupling sites j and $j+1$) within H_A or H_B commute. Thus

$$e^{-i\tau H_B} \approx e^{-i\tau H_1} e^{-i\tau H_3} e^{-i\tau H_5} \ldots$$

So the time evolution operator is a product of individual link terms.

Our DMRG representation of the wavefunction at step i is

$$|\psi\rangle = \sum_{l_{i-1}, s_i, s_{i+1}, r_{i+2}} \psi(l_{i-1}, s_i, s_{i+1}, r_{i+2}) |l_{i-1} s_i s_{i+1} r_{i+2}\rangle$$

Matching the step and the term in the Trotter decomposition, we can apply $e^{-i\tau H_i}$

exactly:

$$e^{-i\tau H_i}|\psi\rangle = \sum_{l_{i-1},s_i,s_{i+1},r_{i+2}} \psi'(l_{i-1},s_i,s_{i+1},r_{i+2})|l_{i-1}s_is_{i+1}r_{i+2}\rangle$$

where

$$\psi'(l_{i-1},s_i,s_{i+1},r_{i+2}) = \sum_{s'_i,s'_{i+1}} \langle s_is_{i+1}|e^{-i\tau H_i}|s'_is'_{i+1}\rangle\psi'(l_{i-1},s'_i,s'_{i+1},r_{i+2})$$

This is expressed in the same basis, and so is exact! Once we have computed ψ', we throw away ψ, and target only ψ'.

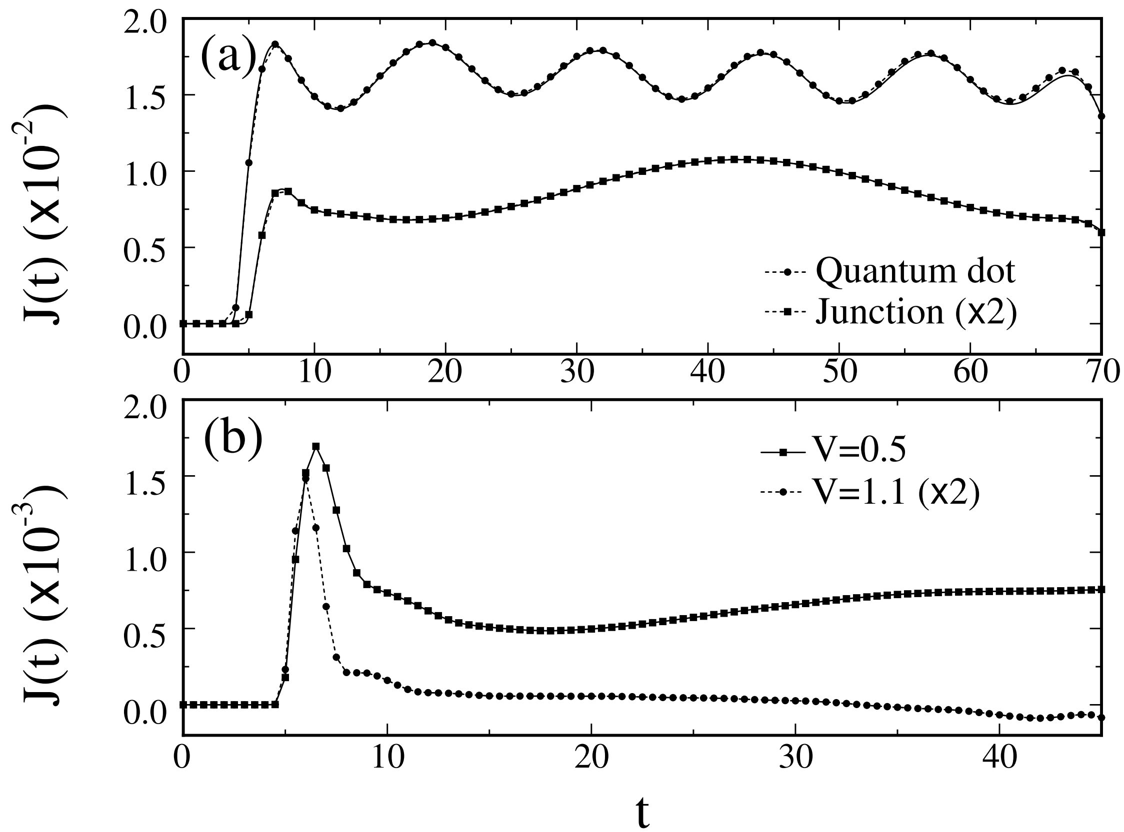
It is convenient to reorder the link terms to match the DMRG sweeps:

$$e^{-2i\tau H} \approx e^{-i\tau H_1}e^{-i\tau H_2}e^{-i\tau H_3}\dots e^{-i\tau H_3}e^{-i\tau H_2}e^{-i\tau H_1},$$

which has the same order Trotter error. Then the time evolution algorithm is almost exactly like the standard finite system DMRG with wavefunction transformations. At left-to-right step i, transform ψ from step $i-1$ to step i, apply $e^{-i\tau H_i}$, and use it to build the density matrix. Applying $e^{-i\tau H_i}$ replaces the usual Lanczos/Davidson step. Each full sweep evolves ψ by 2τ. Aside from the Trotter error, this method is quasiexact, even though it targets only one state!

Tests

Fermion models considered by Cazalilla and Marston: a quantum dot connected to two non-interacting leads, and a junction between two Luttinger liquids, with a sudden voltage bias turned on. These systems are gapless.



Top panel compares with exact results for noninteracting cases; bottom is interacting. The results keeping $m = 128$ states are better than LXW's keeping 512, and much better than Cazalilla and Marston. A small Trotter error is visible in the top panel near $t = 70$.

Calculating Spectral functions

To get spectral functions, we Fourier transform a time dependent Green's function such as

$$G(t) = \langle \phi | B(t) A(0) | \phi \rangle$$

where ϕ is the ground state. Here is the recipe:

- Use standard DMRG to get $|\phi\rangle = |\phi(t=0)\rangle$. Turn off Davidson/Lanczos.

- During a half sweep, apply A to $|\phi\rangle$, $|\psi(t=0)\rangle = A|\phi\rangle$, targetting both ϕ and ψ, and doing the wavefunction step-to-step transformation.

- Start the sweeps to time evolve, applying the link operators, on both $\phi(t)$ and $\psi(t)$.

- Measure $G(t)$ as

$$G(t) = \langle \phi(t) | B | \psi(t) \rangle$$

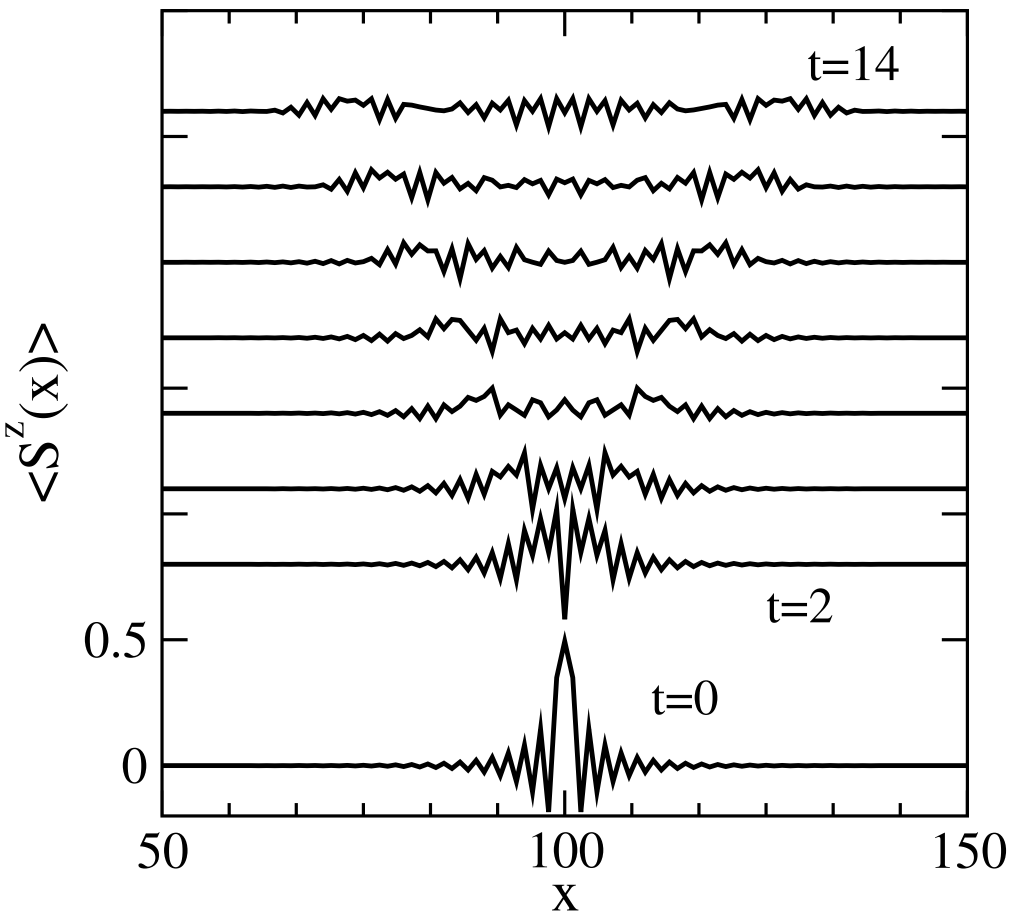
To get all momenta at once, let A be, e.g., S_i^+ for the center site i, and measure with $B = S_j^-$ for all sites j as you sweep. This gives you, for example

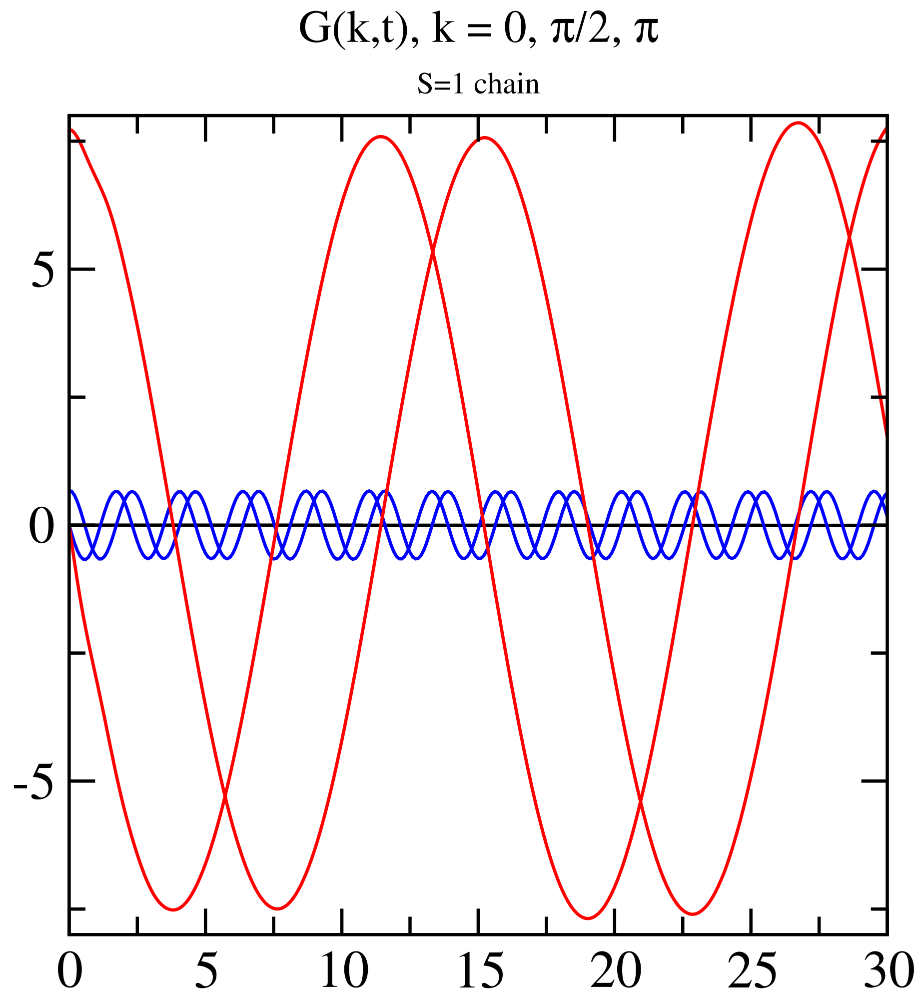
$$G(i-j,t) = \langle \phi | S^-(j,t) S^+(i,0) | \phi \rangle$$

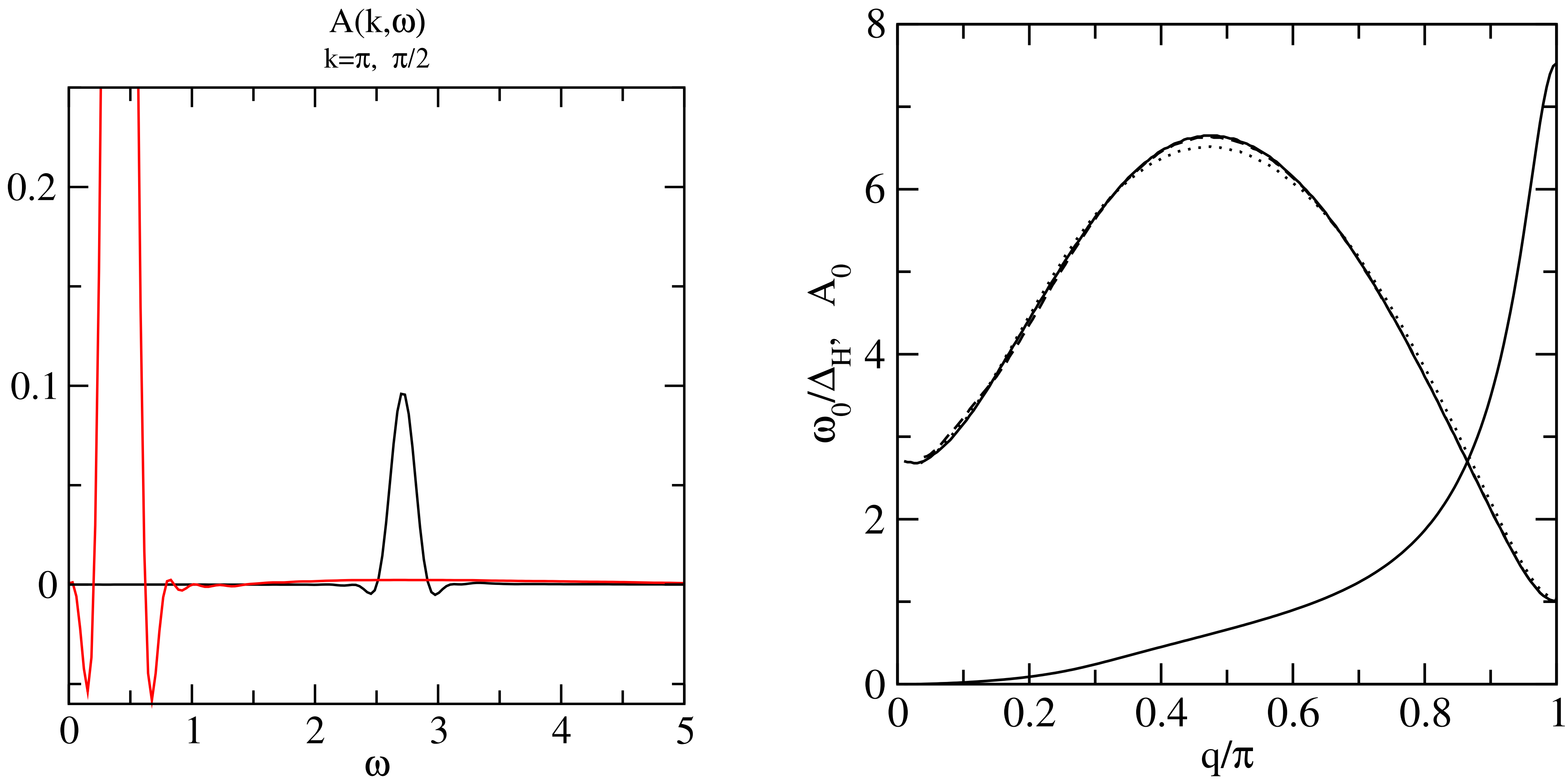
This we can Fourier transform in both space and time to get $G(k,\omega)$.

Example: $S = 1$ Heisenberg chain

To see what the time dependent simulation is doing, here I show $\langle\psi(t)|S^z_j|\psi(t)\rangle$ and $G(k,t)$







S=1 chain, spectral function (left) and dispersion of the quasiparticle peak. On the left, $k = \pi$ and $k = \pi/2$. Changing the FFT procedure can remove the negative regions at the expense of broadening the peaks, $\Delta\omega \sim 1/T$. On the right, location of the main peak is shown for three runs: $[L = 600,\ m = 200,\ \tau = 0.01,\ T = 27.3]$; $[L = 400,\ \tau = 0.05,\ T = 60$, and $m = 150]$; $[L = 400,\ \tau = 0.2,\ T = 72$, and $m = 200]$. Visible errors come from finite τ.

Time-step targetted method

The Trotter methods are very efficient but have two weaknesses:

- The Trotter error. This can be made neglible by using higher-order Suzuki expansions, with e.g. overall errors of order τ^4 instead of τ^2:

$$e^{-i\tau H} \approx e^{-i\tau\alpha_1 H_A} e^{-i\tau\beta_1 H_B} e^{-i\tau\alpha_2 H_A} e^{-i\tau\beta_2 H_B} \ldots$$

  This adds complications but is useful.

- It can't do ladders/2D or beyond nearest neighbor interactions.

To fix these problems Feiguin and I have developed another method, which targets one time step accurately, then moves to the next time step. The time step is similar to that of the Trotter method, e.g. $\tau = 0.1$. The targetting principle is that of Luo, et al. It can be implemented in various ways; we have implemented a Runge-Kutta method.

Recall the fourth order Runge-Kutta method for integrating $y'(t) = f(y,t) = f(y)$:

$$k_1 = \tau f(y); \quad k_2 = \tau f(y + k_1/2); \quad k_3 = \tau f(y + k_2/2); \quad k_4 = \tau f(y + k_3);$$

Then

$$y(t+\tau) \approx y(t) + \frac{1}{6}(k_1 + 2(k_2+k_3) + k_4)$$

Using Mathematica, we find that to $O(\tau^4)$,

$$y(t+\tau/3) \approx y(t) + \frac{1}{162}(31k_1 + 14(k_2+k_3) - 5k_4)$$

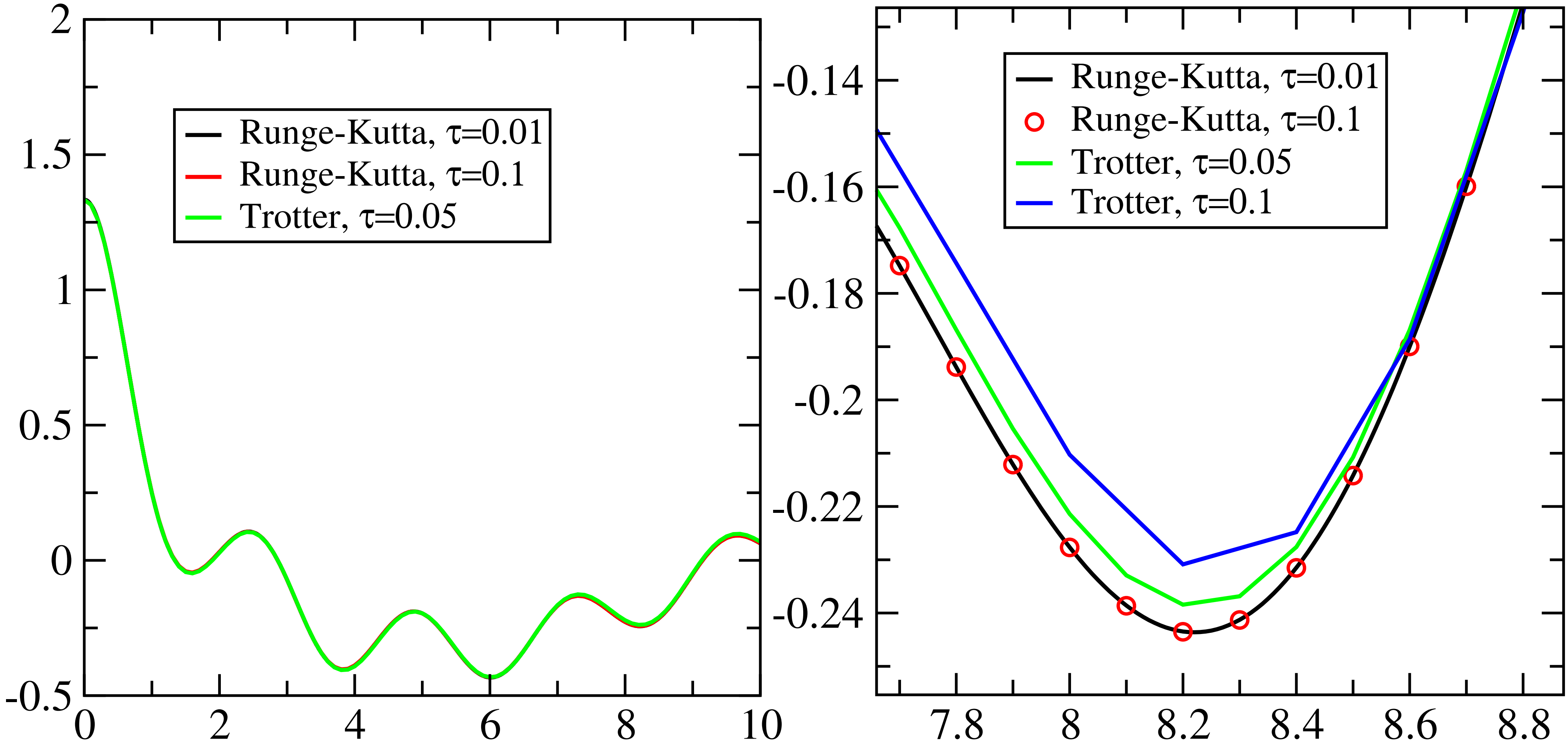
$$y(t+2\tau/3) \approx y(t) + \frac{1}{81}(16k_1 + 20(k_2+k_3) - 2k_4)$$

The recipe is:

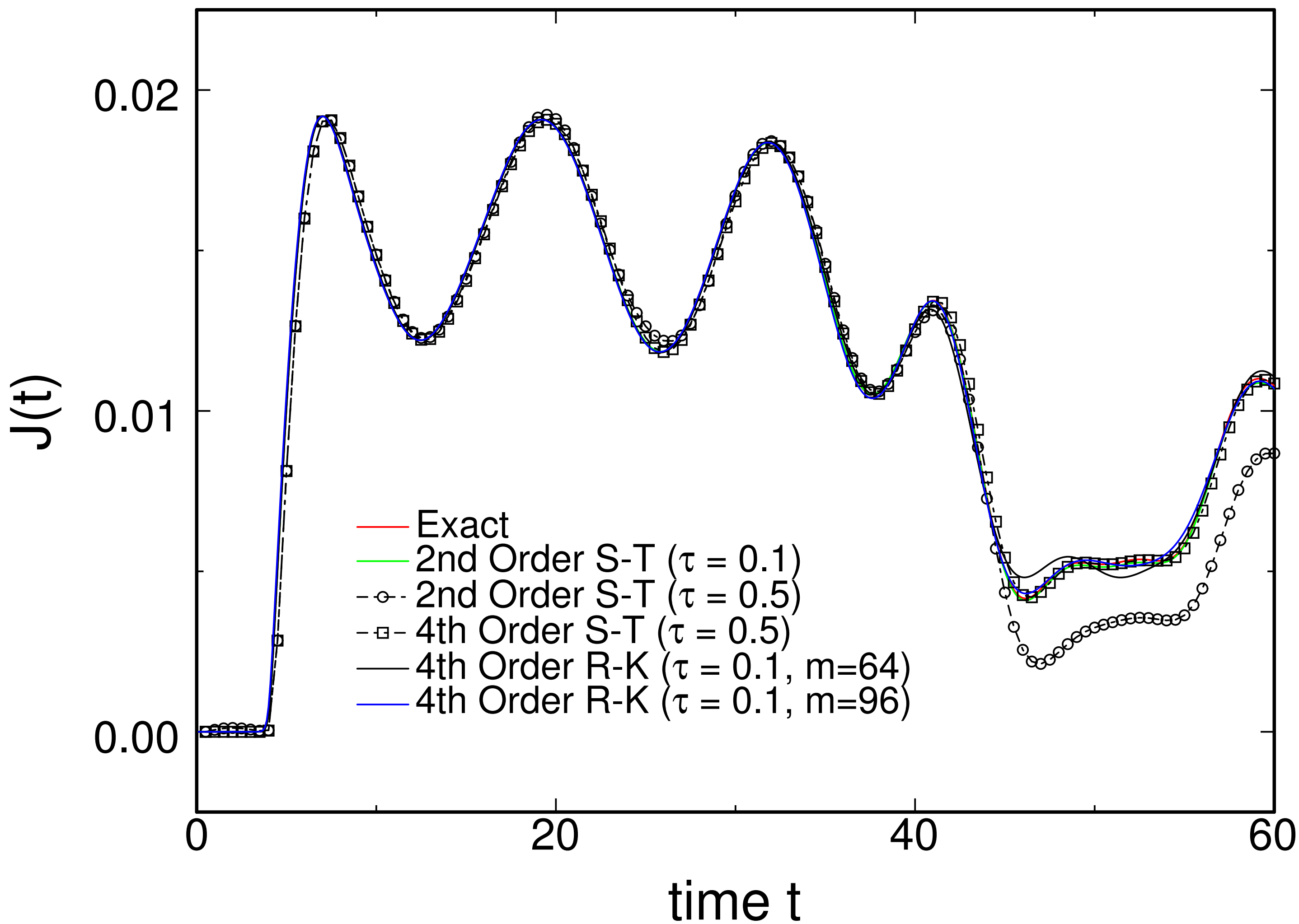
- Each half-sweep is one time step. At each step of the half-sweep, do one RK step, but without advancing $t \to t+\tau$.
- At each step, target $\psi(t)$, $\psi(t+\tau/3)$, $\psi(t+2\tau/3)$, and $\psi(t+\tau)$.
- At the last step, when the basis fully represents the states of the time step, advance to $t+\tau$ more accurately using 10 RK steps with step $\tau/10$.

Comparison: time-step targetted RK method versus Trotter

31 site $S = 1$ Heisenberg chain, $\langle S^{-}(16,t)S^{+}(16,0)\rangle$.



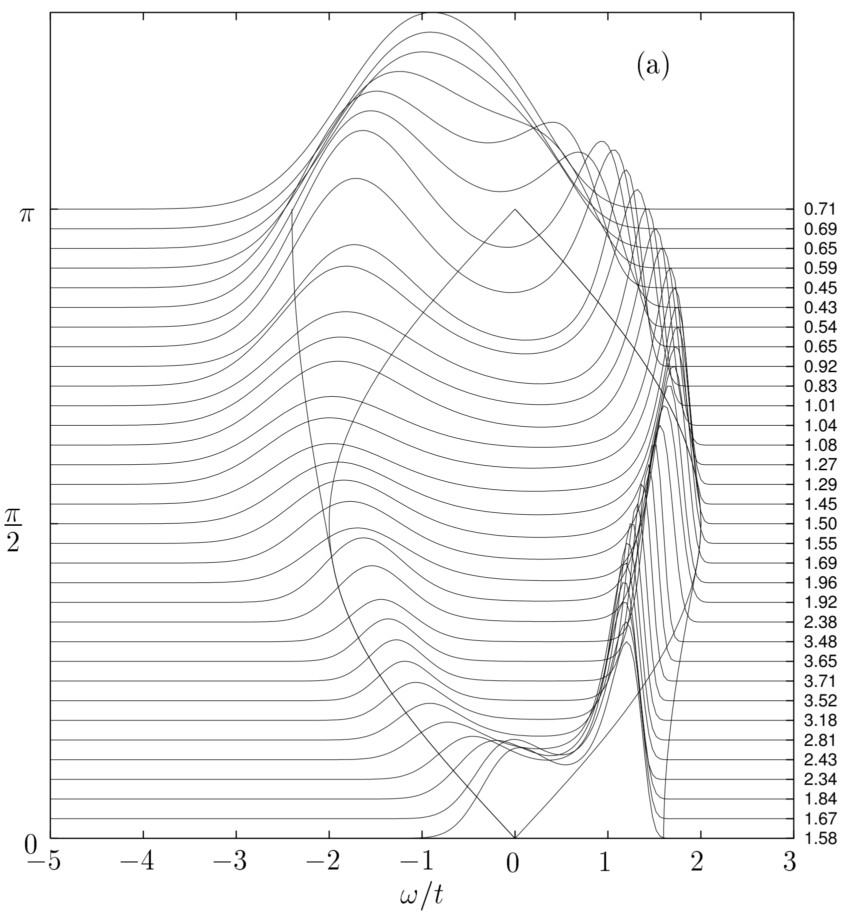
32 site spinless Fermion quantum dot system, exactly soluble, measuring current.

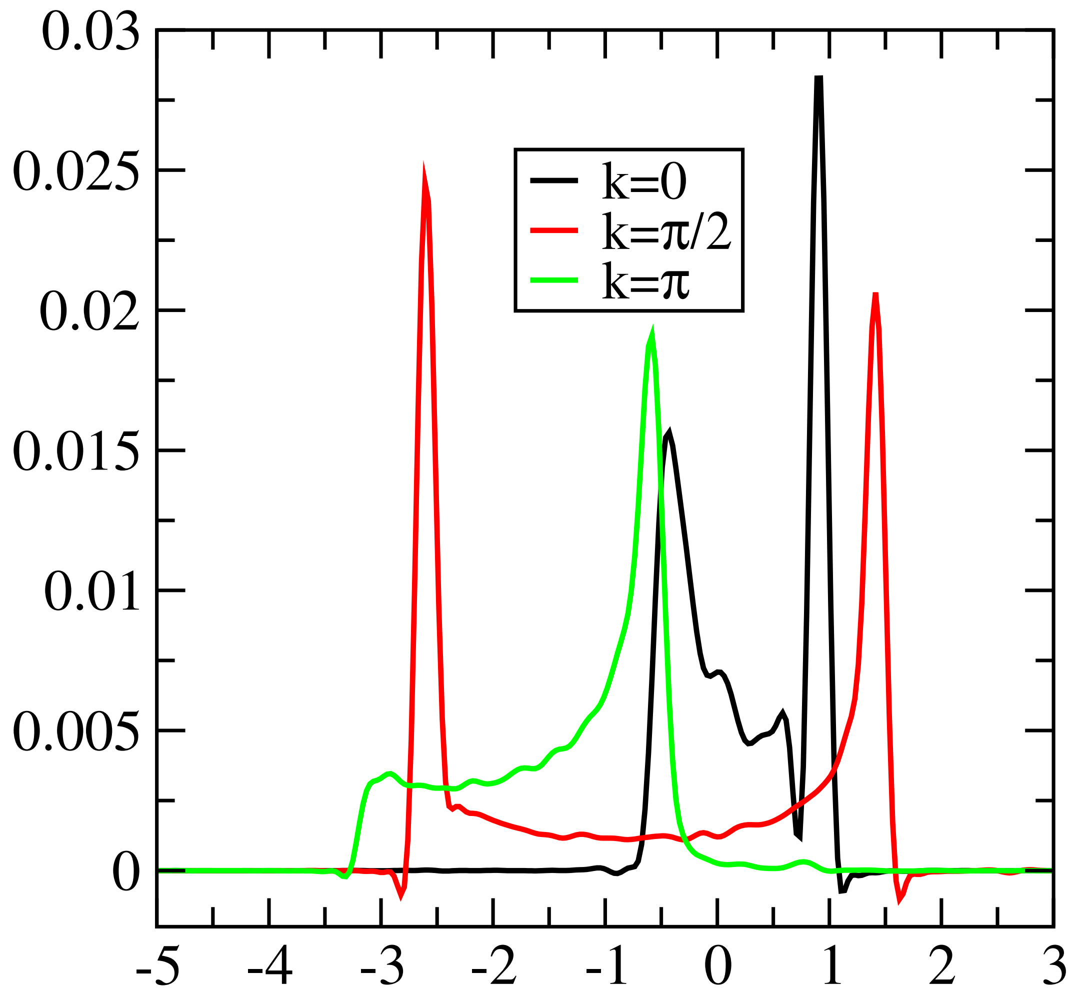


Conclusion: RK method can be very accurate and has no Trotter error.

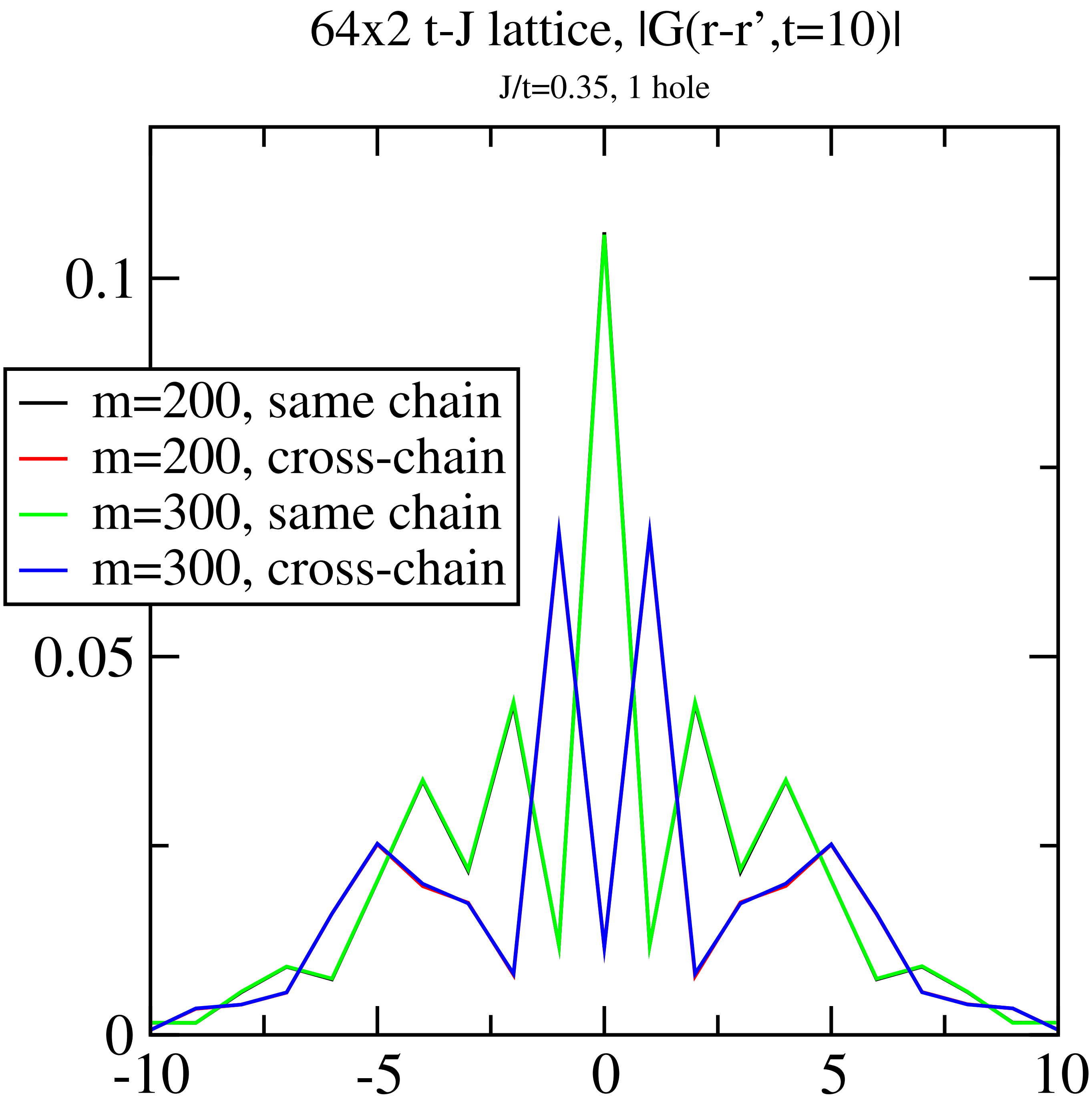
Example system: 1-d t-J model

1D t-J system, spectral weight function for adding one hole to the half-filled (undoped) system. $J = 0.4$. Left hand panel shows results of Brunner, Assaad, and Muramatsu, $L = 64$, using a special quantum Monte Carlo good for one hole and maximum entropy. Right panel is RK method, $L = 200$, $m = 300$, total time $T = 20$.

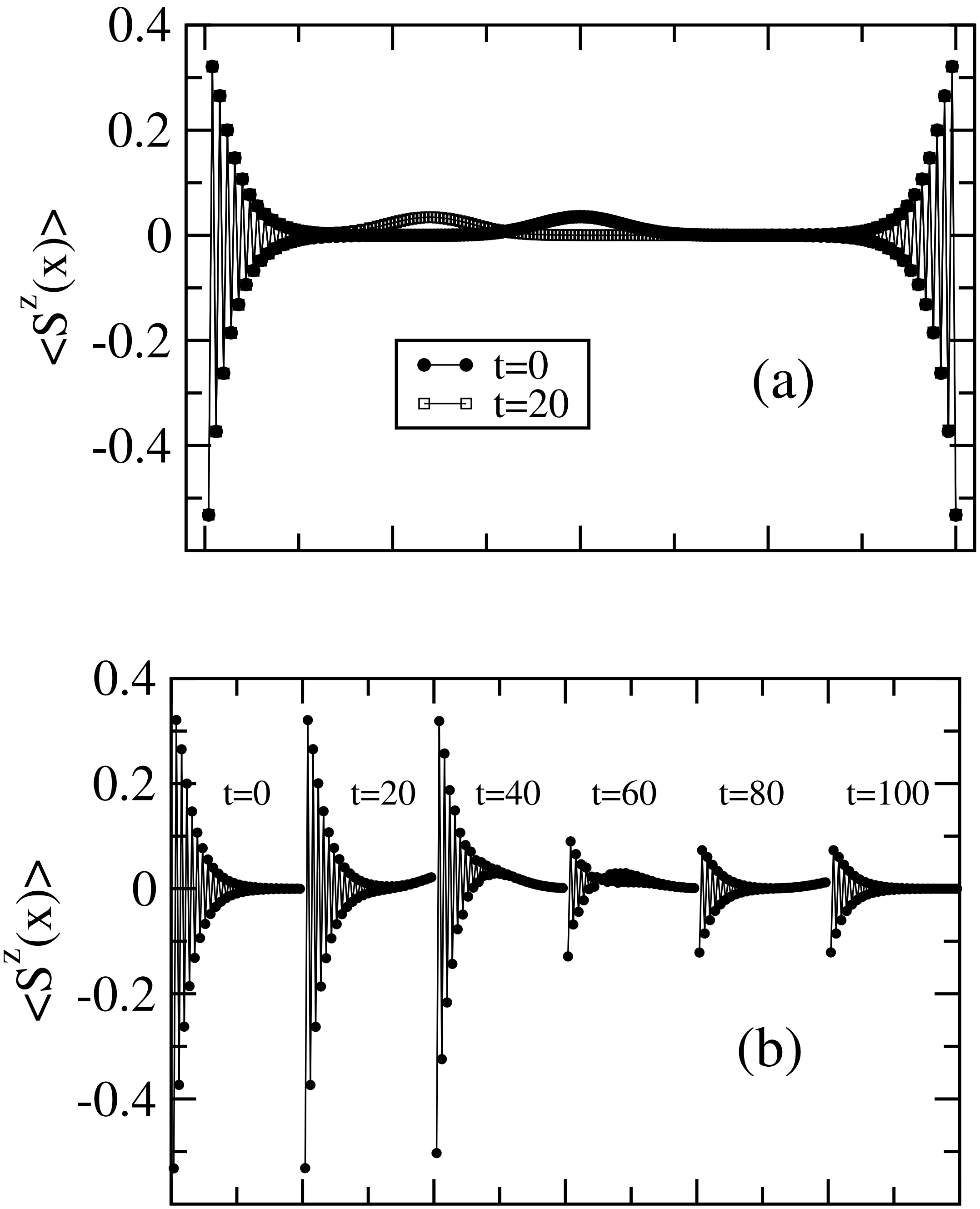


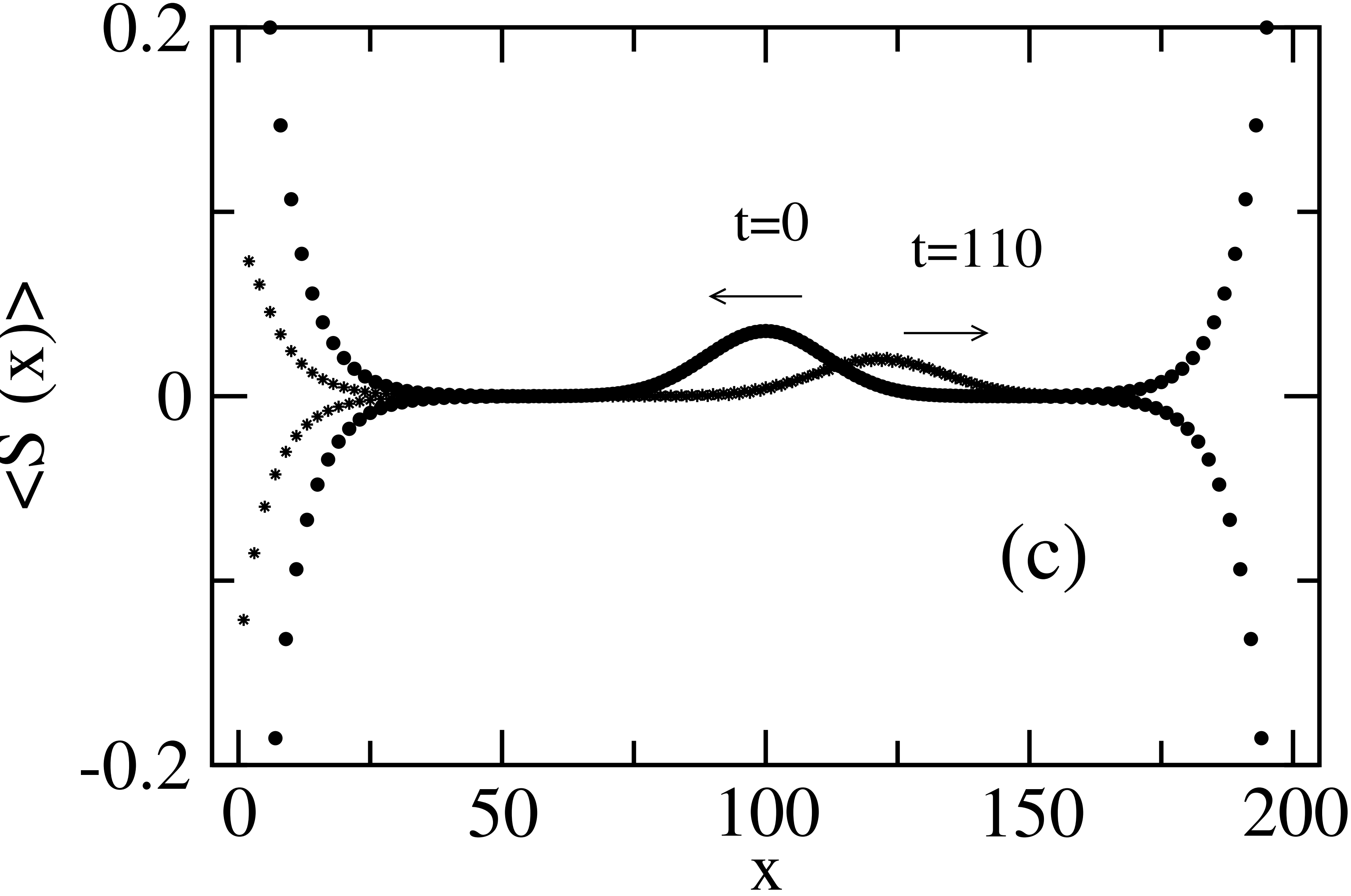


Example system: t-J Ladder



Wavepackets and long-range entanglement in the $S = 1$ chain





0.2
0
-0.2
<S^z(x)>
t=0
t=110
(c)
0
50
100
150
200
x

Conclusions

- If you already know DMRG, and have a good program, time dependent DMRG is easy, fast, and powerful.
- It can give entire spectra much faster than the best frequency methods, and the accuracy is comparable.
- Time dependence can do several key things that frequency methods can't. It is essential for the new finite temperature methods appearing.