Notes on numerical stabilization in determinant quantum Monte Carlo

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In these notes we will empirically compare different matrix decompositions for use in numerical stabilization in many-body quantum Monte Carlo simulation, in particular when calculating equal time Green's functions. We will both benchmark their speed and accuracy. We will further show that special care has to be taken when calculating time-displaced Green's functions and will review a well-known but somewhat hard to find method for stabilizing the necessary inversion in this case. We will focus on and use the Julia programming language for all calculations. An implementation of all discussed methods is available in the open-source software library StableDQMC.jl.

I. THE ISSUE

1. Determinant quantum Monte Carlo in a nutshell

For the description of the DQMC algorithm, we consider a quantum field theory that can be split into a purely bosonic part S_B and a part S_F, which comprises fermion kinetics T and boson-fermion interactions V. An example is the famous Hubbard model after decoupling the on-site interaction $Un_{i,\uparrow}n_{i,\downarrow}$ by means of a Hubbard-Stratonovich or Hirsch transformation in either the spin or charge channel[1]. As per usual, the central quantity of interest is the partition function

$$\mathcal{Z} = \int D\left(\psi, \psi^\dagger, \phi\right) e^{-S_B - S_F} . \tag{1}$$

The basic idea is to switch from the d dimensional quantum theory to a $D = d + 1$ dimensional classical theory as in the path integral framework. The first step is to discretize and Trotter decompose the imaginary time τ,

$$\mathcal{Z} = \int D\phi \; e^{-S_B} \mathrm{Tr}\left[\exp\left(-\Delta\tau \sum_{l=1}^{M} \psi^\dagger \left[T + V_\phi\right] \psi\right)\right] . \tag{2}$$

The exponential is then separated and the appearing commutator ignored which results in a systematic error of the order $\mathcal{O}\left(\Delta\tau^2\right)$,

$$\begin{aligned} e^{A+B} &\approx e^A e^B \\ e^{-\Delta\tau(T+V)} &\approx e^{-\frac{\Delta\tau}{2}T} e^{-\Delta\tau V} e^{-\frac{\Delta\tau}{2}T} + \mathcal{O}\left(\Delta\tau^3\right), \\ \mathcal{Z} &= \int D\phi \; e^{-S_B} \mathrm{Tr}\left[\prod_{l=1}^{m} B_l\right] + \mathcal{O}\left(\Delta\tau^2\right) . \end{aligned} \tag{3}$$

Note that the potential part $e^{-\Delta\tau\psi^\dagger V_\phi \psi}$ in the time-slice propagators $B_l = e^{-\frac{\Delta\tau}{2}\psi^\dagger T \psi} e^{-\Delta\tau\psi^\dagger V_\phi \psi} e^{-\frac{\Delta\tau}{2}\psi^\dagger T\psi}$ depends on the boson ϕ due to the present fermion-boson coupling. Rewriting the trace in (3) as a determinant, an identity which can be proven CITE, yields the fundamental form

$$\mathcal{Z} = \int D\phi \; e^{-S_B} \det G_\phi^{-1} + \mathcal{O}\left(\Delta\tau^2\right), \tag{4}$$

where

$$G = \left(\mathbb{1} + B_M B_{M-1} \cdots B_1\right)^{-1} \tag{5}$$

is the equal-time Green's function.

Only under specific circumstances, such as the presence of a symmetry, can the integral kernel be safely be interpreted as a probability weight, as G_ϕ and its determinant are generally complex valued (*sign problem*).

2. Numerical instabilities

Let us consider the simple non-interacting model system

$$H = -t \sum_{\langle i,j \rangle} c_i^\dagger c_j + \mu \sum_i n_i \tag{6}$$

where we set the hopping amplitude to $t = -1$, the chemical potential to $\mu = -0.1$, and the Hamiltonian has simple tridiagonal form in the position basis.

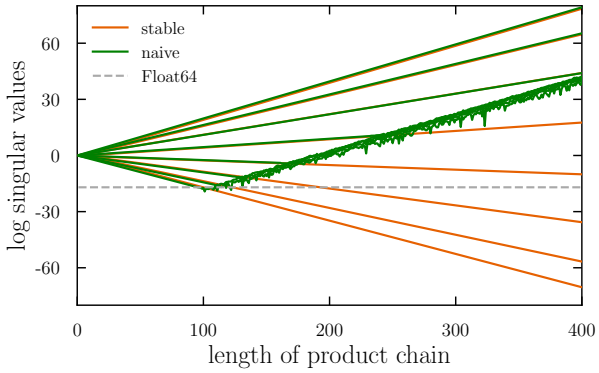

FIG. 1. **Numerical instabilities** (green) due to finite machine precision (Float64) in the calculation of the slice matrix product chain $B_M B_{M-1} \cdots B_1$ for model (6).

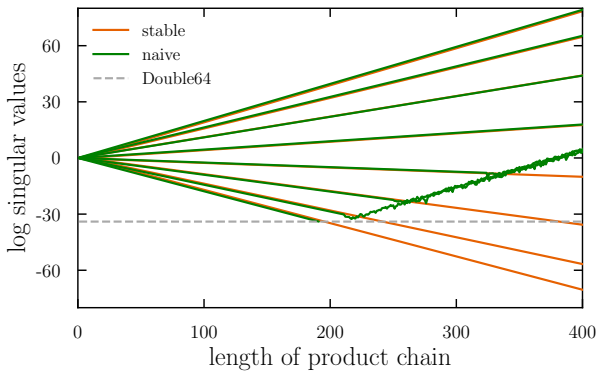

FIG. 2. **Numerical instabilities** due to finite machine precision (Double64) in the calculation of the slice matrix product chain $B_M B_{M-1} \cdots B_1$ for model (6).

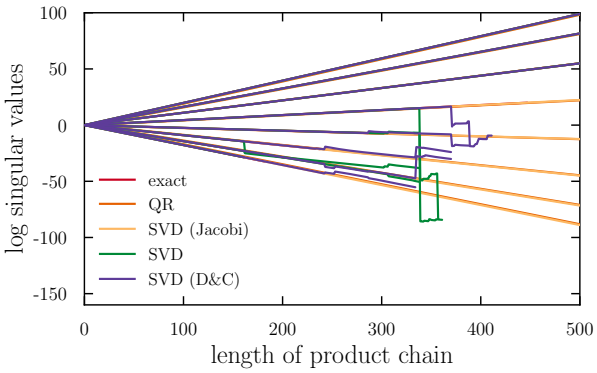

FIG. 3. **Comparison of matrix decompositions** to heal the numerical instabilities in the calculation of the slice matrix product chain $B_M B_{M-1} \cdots B_1$ for model (6). The QR and Jacobi SVD singular values lie on top of the exact ones whereas regular SVD and divide-and-conquer SVD show large deviations at low temperatures $\beta \gtrsim 25$ ($\Delta\tau = 0.1$).

II. MATRIX DECOMPOSITIONS FOR THE RESCUE

Stable multiplication:

$$\begin{aligned} B_2 B_1 &= \underbrace{U_2 D_2 X_2}_{B_2} \underbrace{U_1 D_1 X_1}_{B_1} \\ &= U_2 \underbrace{(D_2((X_2 U_1) D_1))}_{U' D' X'} X_1) \qquad (7) \\ &= U_r D_r X_r, \qquad (8) \end{aligned}$$

with $U_r = U_2 U'$, $D_r = D'$, and $X_r = X' X_1$.

Stable inversion:

$$\begin{aligned} [1 + UDX]^{-1} &= [U \underbrace{(U^\dagger X^{-1} + D)}_{udx} X]^{-1} \qquad (9) \\ &= [(Uu) d (xX)]^{-1} \\ &= (xX)^{-1} d (Uu)^{-1} \\ &= U_r D_r X_r, \qquad (10) \end{aligned}$$

with $U_r = (xX)^{-1}$, $D_r = d$, $X_r = (Uu)^{-1}$.

A. SVD ($UDV^\dagger$)

B. QR (UDT)

III. BENCHMARKS

A. Accuracy

B. Efficiency

IV. THE TIME-DISPLACED GREEN'S FUNCTION

Scalettar and other's method[2] Hirsch method[3]

[1] J. E. Hirsch, "Discrete Hubbard-Stratonovich transformation for fermion lattice models," Physical Review B **28**, 4059–4061 (1983).

[2] E. Y. Loh, J. E. Gubernatis, R. T. Scalettar, S. R. White, D. J. Scalapino, and R. L. Sugar, "Numerical Stability and the Sign Problem in the Determinant Quantum Monte Carlo Method," International Journal of Modern Physics C **16**, 1319–1327 (2005).

[3] J. E. Hirsch, "Stable Monte Carlo algorithm for fermion lattice systems at low temperatures," **38**, 12023 (1988).