The Fermionic Minus-Sign Problem: New perceptions from higher-order Suzuki-Trotter decomposition methods

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Projector Monte Carlo, Suzuki-Trotter decomposition, Hubbard-Stratonovic transformation

Higher order ($p > 2$) Suzuki-Trotter(ST) decompositions with $\sum_{n=1}^{M_{\rm sub}} \gamma_n = \sum_{n=1}^{M_{\rm sub}} \eta_n = 1$,

$$\mathrm{e}^{-\tau(\hat{K}+\hat{U})} = \prod_{n=1}^{M_{\rm sub}} \mathrm{e}^{-\gamma_n \tau \hat{K}} \mathrm{e}^{-\eta_n \tau \hat{U}} + O\left(\tau^{p+1}\right),$$

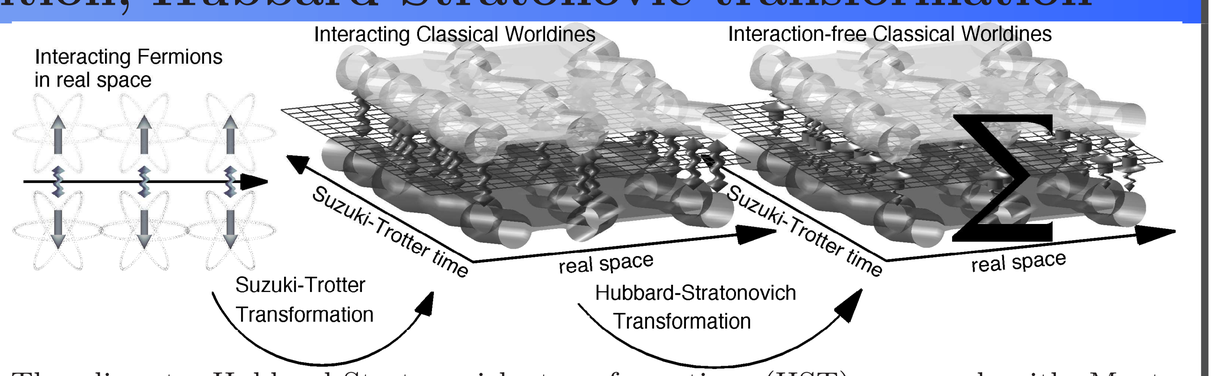
for a time slice τ have been shunned for Quantum Monte Carlo (QMC) as cumbersome and computationally expensive[1]. In projector quantum Monte Carlo (PQMC), the operator $\mathrm{e}^{-\theta\hat{H}}$ 'filters' the ground state $|0\rangle$ from a trial state $|t\rangle$ and exponentially suppresses higher states

$$\mathrm{e}^{-\theta\hat{H}}\,|t\rangle = \mathrm{e}^{-\theta E_0}\,\langle 0|t\rangle \cdot |0\rangle + \sum_{m>0} \mathrm{e}^{-\theta E_m}\,\langle m|t\rangle \cdot |m\rangle$$

With PQMC, we analyze the ground state of the Hubbard Hamiltonian

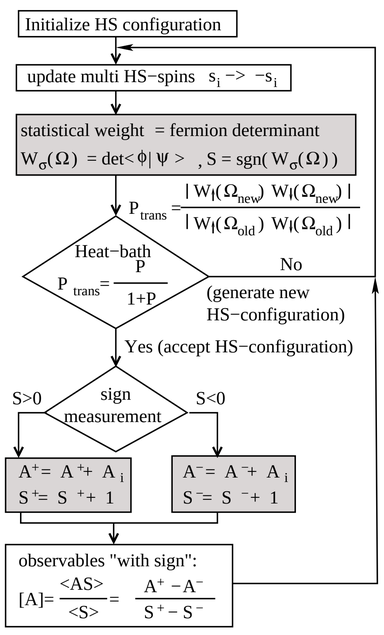
$$\hat{H} = -t \sum_{\langle ij\rangle,\sigma} \left(c^\dagger_{i,\sigma} c_{j,\sigma} + c^\dagger_{j,\sigma} c_{i,\sigma}\right) + U \sum_i n_{i,\uparrow} n_{i,\downarrow},$$

with various orders of ST-decompositions[4], using the correspondence between time-slice-decompositions for symplectic differential equations and operator exponentials[2].

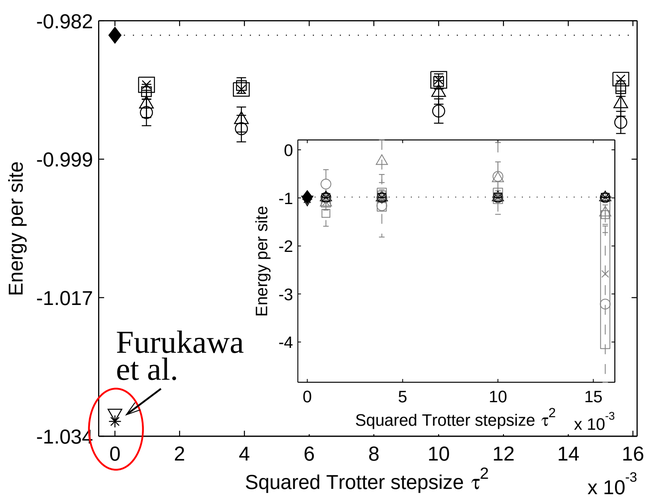


The discrete Hubbard-Stratonovich transformation (HST) summed with Monte-Carlo[5] decouples the interaction. For slices with negative prefactors, the HST for negative U is used[4]. For the resulting Greens-functions, particles cannot be discriminated, in contrast to 'World-line' approaches, where 'individual particle trajectories' in imaginary time are simulated, which violates the principle of indiscriminability of particles in quantum mechanics!

QMC sampling with sign



. . . was first adopted by H. De Raedt *et al.* as 'only a trick'[3] to increase the scattering so that the error-bars fit the theoretical predictions. While in MC and QMC, always positive quantities are used as transition probabilities for the Markov chain, it is now claimed that for the sampling, that the sign must be introduced. For most cases this leads to division by an 'average sign' close to zero, the so-called 'minus-sign problem', hampering the applicability QMC. The sign is reintroduced *ad hoc* after the MC-sampling, which corresponds to a reweighing procedure. The sign was by Furukawa et al [6] due to bad correspondence between PQMC-results without sign and exact diagonalization results, nevertheless, the likely cause was the unstable matrix inversion: we have argued[7] that the 'inclusion of the sign' leads to error compensation, as error-affected measurements have about equal probability to have positive or negative sign. We find consistent results both with and without sign, with better accuracy than Furukawa et al. with 'optimized' test wave functions[6]:



The analytic form of probabilities for single spin-flips shows that negative configurations only occur when local densities for a single Suzuki-Trotter-slice become larger than 1 or smaller than zero: If such unphysical densities are eliminated, the values for sampling with with sign come closer to the values for sampling without sign.

Energies for 4×4 $N_\uparrow = N_\downarrow = 5$ with $U = 8$; $E_{\rm exact} = -1.2238$

Ground state energy for $N_\uparrow = N_\downarrow = 5$ with $U = 4$, computed with Intel extended precision (10 Byte double precision).
Sign $\langle S\rangle \propto \sum_n |\eta_n|$ (cyan), pseudo-symplectic decompositions with only positive coefficients produce $\langle S\rangle \approx 1$ (blue).

Method	p	$\langle E\rangle$sign ignored	$[E]$ with sign	average sign $\langle S\rangle$	$\sum_n \lvert\gamma_n\rvert$ for $\hat{K}$	$\sum_n \lvert\eta_n\rvert$ for $\hat{U}$
Suzuki-Trotter$_1$	1	-1.2418±0.0008	-1.2420±0.0008	0.9954±0.0004	1.0	1.0
McLachlan$_2$	2	-1.2229±0.0008	-1.2232±0.0008	0.9954±0.0004	1.0	1.0
Suzuki-Trotter$_2$	2	-1.2237±0.0008	-1.2240±0.0008	0.9955±0.0004	1.0	1.0
McLachlan$_3$	3	-1.222±0.001	-1.225±0.001	0.952±0.001	1.3760	1.3760
Ruth$_3$	3	-1.205±0.001	-1.225±0.002	0.502±0.004	1.0833	2.3333
Blanes & Moan$_4$	4	-1.201±0.001	-1.223±0.002	0.425±0.005	1.1562	2.4007
Calvo & Sanz-Serna$_4$	4	-1.222±0.001	-1.224±0.001	0.9735±0.0009	1.2811	1.2418
Candy & Rozmus$_4$⋆	4	-1.167±0.002	-1.6±2.3	0.002±0.002	1.7024	4.4048
Chambers$_{4A}$	4	-1.2239±0.0009	-1.2242±0.0009	0.9953±0.0004	1.0	1.0
Chambers$_{4B}$	4	-1.2240±0.0007	-1.2243±0.0007	0.9949±0.0004	1.0	1.0
McLachlan$_4$	4	-1.2234±0.0009	-1.2242±0.0009	0.9838±0.0008	1.4496	1.1716
Suzuki fractal$_4$	4	-1.204±0.002	-1.227±0.002	0.462±0.004	1.4869	2.3159
McLachlan$_5$	5	-1.198±0.001	-1.221±0.002	0.440±0.004	1.4606	2.3833
Tselios$_5$⋆	5	-1.225±0.004	-1.4±0.3	-0.000±0.001	1.9717	10.8147
Blanes & Moan$_{6A}$	6	-1.217 ±0.001	-1.223±0.001	0.860±0.003	2.0118	1.6592
Blanes & Moan$_{6B}$	6	-1.200 ±0.002	-1.225±0.003	0.372±0.004	1.2061	2.4935
Chambers$_{6A}$	6	-1.2229±0.0008	-1.2231±0.0008	0.9949±0.0004	1.0	1.0
Chambers$_{6B}$	6	-1.2252±0.0008	-1.2257±0.0008	0.9941±0.0005	1.0	1.0
Yoshida$_{6A}$⋆	6	-1.158±0.003	-0.8±0.6	0.002±0.001	2.8842	5.7107
Laskar & Robutel$_{8A}$	8	-1.2236±0.0008	-1.2240±0.0008	0.9945±0.0005	1.0	1.0
Yoshida$_{8D}$⋆	8	-0.878±0.005	-2.0±1.2	-0.000±0.004	10.3491	15.2548

Errors for $\exp(-\theta H)$, H

While the error for decompositions of $\exp(-\theta H)$ is well known, t the accuracy of the observables is LOWER. In the case of the Hamiltonian H, the accuracy is

$$H = H_A + H_B + \underbrace{\frac{\tau}{2}\{H_A, H_B\}}_{\rm error} + O(\tau^2),$$

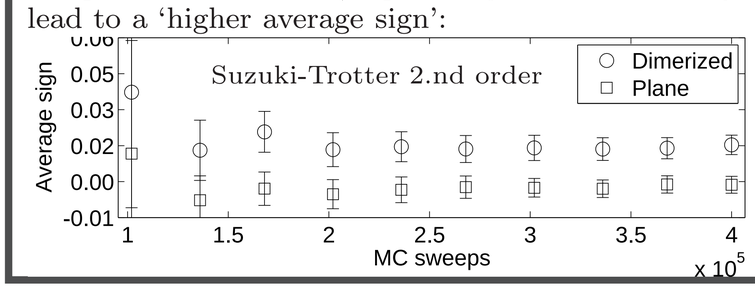
with the anti-commutator $\{\cdot\}$, one order lower than for $\exp(-\tau H)$[8]. For a first-order approximation of the exponential, the Hamiltonian is of zeroth order, which is independent of τ ! In 2nd order, one has[8]

$$H = H_A + H_B + \underbrace{\frac{\tau^2}{12}\left\{\{H_A, H_B\}, H_B + \frac{1}{2}H_A\right\}}_{\rm error} + O(\tau^4).$$

a.s.o. for higher order[9]. Due to the commutators in the error term, PQMC does not converge uniquely 'from above' or 'from below' to the ground-state energy.
We have focused on the Energy, as the Hohenberg-Kohn theorem states that the energy is a unique functional of the electron densities: If the energies are wrong, the electron densities are also wrong, and the computation of other quantities is meaningless.
Suzuki-Trotter$_1$ (first order) deviates much from $E_{\rm exact}$ even with reasonable $\langle S\rangle$ (magenta): This shows that zero-order for H for first order of $\exp(-\tau H)$, is realistic. The sign decays with the absolute sum of the Suzuki-Trotter-timesteps $\sum_n |\eta_n|$ for the interaction U.
While for 'exact' Suzuki-Trotter decomposition for order 3 or higher, at least one slice must be negative, 'pseudo-symplectic' decompositions allow purely positive slices with $\sum_n |\eta_n| = 1$, with 'benign' sign.

Influence of the test function

For different test wave functions, we get different sign, which shows that the sign is a not a quantity which depends on the decomposition alone. 'More symmetric' decomposition formulae (respectively HS-fields in PQMC) lead to a 'higher average sign':



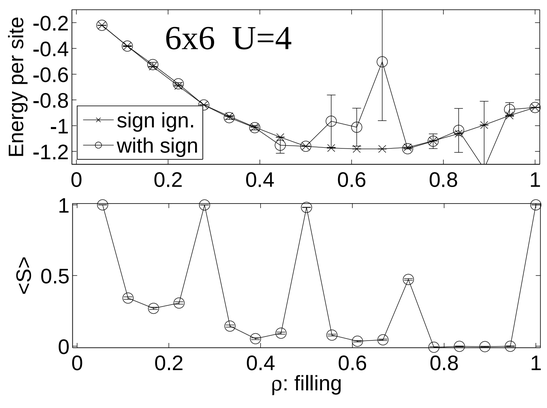
Summary and Conclusions

Whether $[E]$ gives results closer to $E_{\rm exact}$ depends on the physical parameters. Negative fermion determinants can be attributed to the loss of symmetry in the product matrix of itself symmetric matrices, i.e. asymmetry of ST-product with the potentials of the auxiliary field method.
The determinant quantum Monte-Carlo methods make extensive use of linear algebra. In the past, unstable matrix-inversion and orthogonalizations have been used; In the case of 'samling with sign', the numerical errors were distributed between 'positive' and 'negative' configurations. The resulting error compensation was mistaken as a 'success' and justification of the minus-sign method. There is no theoretical argument why the sign should be included in the sampling:

1) The sign varies by orders of magnitude depending on the Suzuki-Trotter decomposition, so it is not a physical observable and has no place in the observable computation.
2) Including the sign corresponds to a reweighing procedure, and there is no argument in MC that reweighing is obligatory: Reweighing is in the choice of the programmer, to obtain more accurate results, not to make simulations impossible.
3) For each configuration, the sign of the determinant depends on the sign of all singular values (SV) of the Fermion matrices, while the observables depend on the largest ones: The error introduced by the Suzuki-Trotter decomposition $O(\tau^{p+1})$ is much larger than the one by changing the smallest Eigen-(Singular-)value of $\exp(-\theta H)$.
4) The unphysical correlation $\langle AS\rangle$ in $[A] = \langle AS\rangle/\langle S\rangle$ can for some systems actually lead to estimates for the energy which are much further off the plausible values than $\langle A\rangle$ itself.

6×6 systems

While for 4×4-systems, 'reweighing' gives 'only larger error bars', for 6×6 systems the results are downright implausible (Note that the error bars are computed via the standard deviation, which assumes normal distributed samples, while the actual scattering between individual simulation results is actually much smaller): This shows that the $[A] = \langle AS\rangle/\langle S\rangle$ is actually an unphysical correlation, and $\langle A\rangle$ is the true observable value.



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