International Journal of Modern Physics C
Vol. 16, No. 6 (2005) 1–10

World Scientific
www.worldscientific.com

NONEXISTENCE OF *d*-WAVE-SUPERCONDUCTIVITY IN THE QUANTUM MONTE CARLO SIMULATION OF THE HUBBARD MODEL

HANS-GEORG MATUTTIS

Department of Mechanical Engineering and Intelligent Systems
The University of Electro-Communications
Chofu, Chofugaoka 1-5-1, Tokyo 182-8585, Japan
hg@mce.uec.ac.jp

NOBUYASU ITO

Department of Applied Physics, School of Engineering
The University of Tokyo, Bunkyo-ku, Tokyo 113-8646, Japan
ito@ap.t.u-tokyo.ac.jp

Received 6 December 2004
Revised 14 December 2004

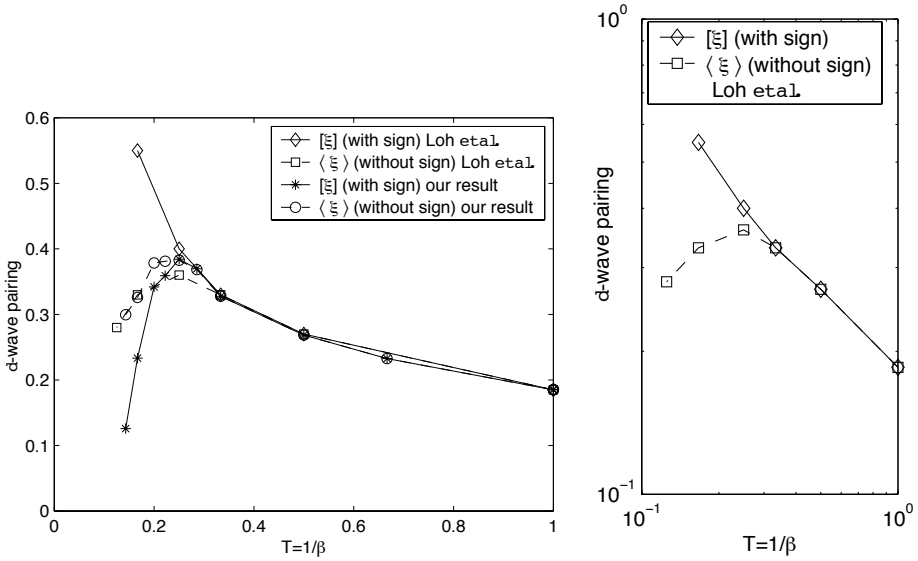
For the existence of *d*-wave-superconductivity in the Hubbard model, previous quantum Monte Carlo results by other authors, which showed a power law increase of the *d*-wave susceptibility, seem to contradict a recently published theorem. We show those quantum Monte Carlo calculations were numerically contaminated, analyze the numerical problem and propose a numerically more stable computing scheme.

Keywords: Hubbard model; minus sign problem; grand canonical quantum Monte Carlo; Hubbard–Stratonovich transformation.

1. Introduction

In a re-investigation of the ground state projector quantum Monte Carlo (PQMC) algorithm, the authors had shown that the bad quality of numerical routines could influence the outcome of quantum Monte Carlo simulations[1] so that numerical errors mimic a "sign problem". Among other things, for numerically accurate algorithms, the sign could be ignored for the sampling of equal-time quantities, i.e., observables computed with and without sign gave identical results within Monte Carlo error-bars. In this paper, we focus on the problem whether and how numerical schemes can affect the outcome of simulations for the finite temperature auxiliary field algorithm[5] and how observables computed from nonequal time Greens functions are affected by the sampling with and without sign.

We wanted to re-investigate the 4×4-Hubbard system (Hubbard-Interaction $U = 4$ and electron filling $\langle n \rangle = 0.875$) in Loh *et al.*[2] for which an increase of the



(a) (b)

Fig. 1. Linear plot for the d-wave pairing susceptibility versus temperature with and without sign of the fermion determinant, (a) results from Loh *et al.* and our results, and (b) double logarithmic plot for the results by Loh *et al.* The size of the error bars for our result are of the size of the symbols or smaller.

d-wave susceptibility was found when the minus sign was taken into account, and a decrease of the susceptibility when the sign was ignored, to understand the influence of the minus sign sampling on time dependent quantities. The power law increase of the d-wave susceptibility, i.e., the response function of the order parameter, towards zero temperature in Loh *et al.*[2] (see Fig. 1) would indicate a critical state, i.e., as a transition to d-wave superconductivity for the given parameters. Loh *et al.*[2] did not dare to draw such a conclusion explicitly and also avoided to publish their data on a logarithmic scale.

A recent theorem by Su *et al.*[3] proves that the two-dimensional Hubbard Model cannot exhibit d-wave pairing for finite temperatures, which is in contradiction to the Monte Carlo results cited above. We decided to re-investigate the result of Loh *et al.* because any contradiction of simulation data with exact theorems is suitable to cast doubt on the reliability of the quantum Monte Carlo method as a whole. On the other hand, the results by Loh *et al.* seemed to be rather dubious, because the increase in the correlation functions is conclusive only for the last two data points, which were used to argue that the sampling with sign and no sign gave different results, whereas the inevitable conclusion from these data points, that the ground state was superconducting with d-wave pairing, was conspicuously avoided.

2. The Grand Canonical Quantum Monte Carlo Method

The grand canonical quantum Monte Carlo method[5] computes directly the equal time Greens function for finite fermionic systems at finite temperatures. The non-commuting kinetic part $\hat{T}$ and the interaction part $\hat{U}$ of the Hamiltonian $\hat{U} = \hat{T} + \hat{U}$ are decoupled using the Suzuki–Trotter (ST) decomposition[6–8] of second order:

$$e^{\tau H} = e^{\hat{T}\tau/2} e^{\hat{U}\tau} e^{\hat{T}\tau/2} + \mathrm{O}(\tau^3)\,. \tag{1}$$

The interaction $\hat{U}$ in $e^{\hat{U}\tau}$ is decoupled using the discrete Hubbard–Stratonovich (HS) transformation[9]

$$e^{-\tau n_\uparrow n_\downarrow} = \frac{1}{2} \sum_{s=\pm 1} e^{2\lambda s(n_\uparrow - n_\downarrow) - \tau/2(n_\uparrow + n_\downarrow)}\,, \tag{2}$$

with $\lambda = \tanh^{-1} \sqrt{\tanh(U\tau/4)}$ for each lattice site, so that the interacting system is simulated by sampling Slater-determinants of interaction-free electrons. According to the configuration S of HS spins s_i at a given site i, the potentials $V(S)_\sigma$ fluctuate in space and time during the Monte Carlo process. The electron density is controlled by introducing a chemical potential μ. The Trotter slice with the HS-decoupled interaction and the hopping-matrix K is then

$$B_{i\sigma}(S) = e^{K\tau/2} e^{V(S)_\sigma} e^{K\tau/2}\,. \tag{3}$$

The equal time Greens function $G(0)$ is computed from the Trotter slices $B_{i\sigma}(S)$ as

$$G(0) = \left(1 + \prod_{i=1,m} B_{i\sigma}\right)^{-1}\,. \tag{4}$$

The nonequal time Greens functions are given in Eqs. (3.25) and (3.26) by Hirsch[5] as

$$G(k\tau) = G(0) B_1^{-1} \cdots B_k^{-1}\,, \tag{5}$$

$$G(-k\tau) = B_k^{-1} \cdots B_1^{-1} (\delta_{ij} - G(0)^T)\,. \tag{6}$$

Because the product of the $B_{i\sigma}(S)$ contains exponentially diverging numerical scales, a "stabilization" in the accumulation of the Trotter product is necessary for the finite-precision floating point arithmetic, otherwise the relevant information drops out due to rounding. When the transition probability becomes negative in the quantum Monte Carlo simulation, its absolute value is used for the Monte Carlo sampling, and the sign S is treated as an observable. Denoting with $\langle \cdots \rangle$ the sampling average during the simulation (from here on called "without sign"), and $[\cdots]$ the thermal expectation value, the average of a physical quantity A are conventionally computed (from here on called "with sign") as

$$[A] = \frac{\langle AS \rangle}{\langle S \rangle}\,. \tag{7}$$

3. *d*-Wave Pairing

The simulations were performed for the two-dimensional Hubbard–Hamiltonian

$$H = \hat{T} + \hat{U}\,, \tag{8}$$

$$H = -t \sum_{\langle i,j\rangle,\sigma} c^{+}_{i\sigma} c_{j\sigma} + \text{h.c.} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}\,, \tag{9}$$

where $c^{+}_{i\sigma}(c_{i\sigma})$ creates (annihilates) a fermion with spin σ on site i. The hopping parameter and the strength of the on-site Coulomb-repulsion are denoted by t and U, respectively. In Loh *et al.*,[2] for the two-dimensional 4×4 Hubbard model with nearest-neighbor hopping at $U = 4$ and $\langle n\rangle = 0.875$ the values for the d-wave pairing susceptibility $[\xi]$ "with sign" were different from the values $\langle\xi\rangle$ "without sign" (reproduced in Fig. 1). Since for $[\xi]$ a power law increase for $T \to 0$ was observed, which was absent in $\langle\xi\rangle$, it was conjectured by Loh *et al.*[2] that qualitative, not only quantitative differences could result in quantum Monte Carlo simulations if the sign was ignored. Reference data to prove which of $[\xi]$ or $\langle\xi\rangle$ were physically accurate were missing, and, to our knowledge, do not exist.

Moreover, the value of $[\xi]$ at $\beta = 8$ was missing, so only two data points corroborated the power law increase for $[\xi]$ at low temperatures, the one at $\beta = 6$ having already error bars of more than 5% of the total value. Neither a value nor an error bar for $[\xi]$ at $\beta = 8$ were given, nor an rationale why for the lowest temperature the value for $[\xi]$ was left out from the graph, whereas the value of $\langle\xi\rangle$ plotted. Data points for $\langle\xi\rangle$ and $[\xi]$ should have been generated by one and the same program run for any given temperature. Moreover, the power law increase of $[\xi]$ for $T \to 0$ at face value should be interpreted as the onset of a superconducting transition, a conclusion Loh *et al.*[2] did not dare to draw.

In other words, the whole argument for the different outcome of sampling with and without sign hinges on two data points, from which the (at the time) "politically convenient" conclusion was drawn that the values for sampling with and without sign gave different results. The other, inevitable conclusion from these data points, that the model showed d-wave superconductivity, was avoided as it would have been "politically precarious" at the time time of the publication, and plainly wrong in today's standard of knowledge.[3,4]

As we had found[10] serious numerical problems (see Appendix 1) with the stabilization scheme Loh *et al.* had proposed in Ref. 11, and as also another work on the discrepancy for observable computations with and without sign[12] turned out to be not sustainable in the light of a numerically more thorough investigation,[1] we suspected serious numerical problems as the ultimate reason for the discrepancy between $[\xi]$ and $\langle\xi\rangle$. We had already devised an improved stabilization scheme (see Appendix B), which we used in the investigation of the two-dimensional attractive Hubbard model,[13] and which we use here for the re-investigation of the d-wave pairing.

The comparison between our results and those of Loh *et al.*[2] are shown in Fig. 1. For $\beta < 3$, our results are in good agreement with the one by Loh *et al.*[2] For our simulation, at $\beta = 4$ the values for $\langle\xi\rangle$ and $[\xi]$ still agree, whereas $\langle\xi\rangle$ and $[\xi]$ already diverge for the results by Loh *et al.*[2] For our simulation, deviations between $\langle\xi\rangle$ and $[\xi]$ developed only below $T = 1/4.5$, and increase monotonically with decaying temperature. Nevertheless, in contrast to Loh *et al.*,[2] both $[\xi]$ and $\langle\xi\rangle$ decay and no power law or otherwise increase can be seen; no qualitative difference is visible between $[\xi]$ and $\langle\xi\rangle$, only a quantitative one. We confirmed our approach numerically by comparing runs with double and quadruple precision (64 and 128 bits), which would have revealed any deficiencies in the stabilization algorithm. Within statistical error bars, data for the Greens functions computed with double and quadruple precision were consistent, only the chemical potential had to be adapted by up to two percent at temperatures below $\beta = 4.5$ to obtain the same filling. Observables computed from equal time Greens functions like energies etc. for this, as well as for other systems[14] did not show any deviations if sampled with or without sign down to the lowest temperatures.

4. Conclusions

We have shown that previous approaches to the numerical stabilization in the grand canonical quantum Monte Carlo simulation can produce spurious results and we have devised a new, improved stabilization scheme (Appendix B). All results and conclusions of authors who used the error-prone stabilizations can be considered unreliable at the least, and totally wrong at the worst, both with respect to observable computations as well as with respect to the conclusions concerning the minus-sign problem.

In contrast to previous investigations,[2] with our improved stabilization, we find no increase of the d-wave superconducting susceptibility towards the ground-state in accordance with the exact results by Su.[3,4] The reliability of the auxiliary field quantum Monte Carlo method as a controllable approximation is out of question. The enhancement of d-wave pairing reported in other quantum Monte Carlo simulations[15] is currently under investigation.

Quantities sampled from nonequal time Greens functions showed quantitative, but no qualitative differences for low temperatures in the case where the sign was ignored or taken into account. Quantities sampled from equal times Greens functions agreed for sampling with and without sign within the statistical error bars, as in the case for the ground state algorithm.[1] The reason for this apparant paradox will be explained in a future publication.

Acknowledgments

We would like to thank P. Pattnaik, R. Natarajan and I. Morgenstern for helpful discussions. One of the authors (H.-G. Matuttis) is grateful for financial support of the Fellowships of the Japan Society for the Promotion of Science for Foreign

Researchers and the Inoue Foundation in Japan. This work was partially supported by the Grant-in-Aid for Scientific Research of Ministry of Education, Science and Culture, Japan.

Appendix A. Previous Stabilizations

A.1. *Equal time Greens functions*

The numerical information contained in a Trotter-product is contained in the full spectrum of its singular values, which widens exponentially with the Hubbard-interaction U and Trotter-time/inverse temperature β. Due to rounding errors, the numerical information can get lost during the accumulation of the Trotter-product.

Stabilization by orthogonalization[11] tries to avoid this by decomposing the Trotter-product into a product of an orthogonal matrix, a diagonal matrix and a third matrix which depends on the numerical decomposition scheme. The separation of numerical scales in the diagonal matrix must be retained up to the inversion step of the Greens function computation in Eq. (4). If the diverging scales are only separated during the accumulation of the product, but are "mixed" into the data before inversion due to an unsuitable order of the numerical operations, the matrix multiplication is stabilized, but the inversion step is still plagued with numerical inaccuracies.

For a HS-spin configurations which is "ferromagnetic" in the imaginary time direction and "anti-ferromagnetic" in the spatial direction, the HS-configuration

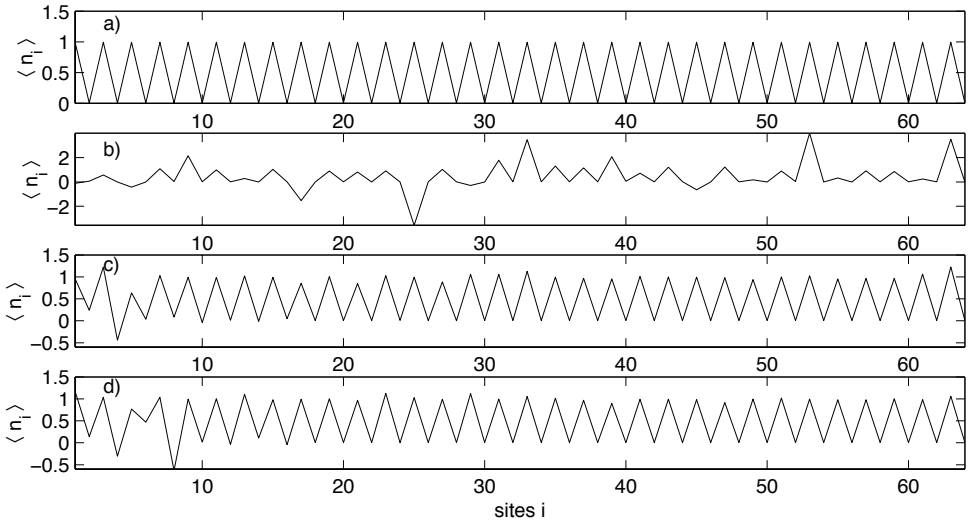


Fig. A.1. Floating point computation result of the diagonal elements of a Greens function (electron densities) for the HS-configuration explained in the main text for a 64 site/8 × 8 system, $\beta = 12.5$, $d\tau = 0.125$, $U = 8$, $\mu = U/2$ with 25 stabilization steps, showing the results for (a) QR decomposition with pivoting/exact result, (b) SVD, (c) MGS and (d) QR decomposition without pivoting.

and therefore the densities $\langle n_i \rangle$ are the same for all "even"/"odd" sites respectively due to symmetry reasons, see Fig. A.1(a), after Matuttis.[10] We tried singular value decomposition (SVD), modified Gram Schmidt (MGS) which were both proposed by Loh *et al.*[11] for this purpose, and QR decomposition after Householder without pivoting (QRH), which is the standard operation for orthogonalizations in the numerical literature.

For our test-case, for the stabilization schemes proposed by Loh *et al.*[11] all results are abysmal, as neither the symmetry in the HS-configuration, nor the positivity in the electron density are conserved (densities for electrons smaller than 0 or larger than 1 beyond the bounds set by the Suzuki–Trotter-decomposition are unphysical). The bad quality of the stabilization schemes using SVD and MGS can be simply understood from the accuracy of the decomposition scheme, which is proportional to the condition number κ of the decomposed matrix in the case of SVD and proportional to the norm of the decomposed matrix in the case of MGS.[17] As the singular values in the decomposed matrix are exponentially large in quantum Monte Carlo runs for low temperatures, both decomposition schemes are unsuitable because exponentially large errors have to be expected.

The results for the QRH-transformation are much better, but without pivoting, in the kernel $(D^{-1} + R^{-1}Q^{-1})$ the entries of D are exponentially distributed, but not ordered. The Greens function

$$G(\tau,\tau) = R^{-1}(Q^{-1}R^{-1} + D)^{-1}Q^{-1}\,, \tag{A.1}$$

(Eq. (3) in Loh *et al.*[11]) has no structure like diagonal dominance etc., which could be exploited for improving the accuracy of the inversion. Large diagonal elements would guarantee numerical stability, as in case of the LU-type of the numerical matrix inversion, where large diagonal elements are enforced via "pivoting".

The numerical usefulness of the QRH-decomposition is still doubtful: spuriously larger diagonal elements will improve the numerical accuracy for some entries of the Greens function in the inversion process, whereas spuriously smaller diagonal elements will introduce errors in other elements. No reliable stabilization effect can be expected, as documented by the occurrence of spuriously negative electron densities in our test case (see Fig. A.1(d)).

A.2. *Nonequal time Greens functions*

Alternative stabilization schemes were proposed by Loh *et al.*[11] for the computation of equal time Greens functions and nonequal time Greens functions alike via

$$G(\tau,\tau) = (U_L^{-1}U_R^{-1} + D_L^{-1}V_L^{-1}U_R^{-1}D_R^{-1})^{-1}\,, \tag{A.2}$$

(Eq. (5) in Loh *et al.*[11]) and

$$G(\tau,0) = U_L D_L V_L (1 + U_L D_L V_L U_R D_R V_R)^{-1}\,, \tag{A.3}$$

$$G(\tau,0) = V_R^{-1}(D_L^{-1}U_L^{-1}V_R^{-1} + V_L V_R D_R)^{-1}V_L^{-1}\,, \tag{A.4}$$

(Eq. (7) in Loh *et al.*[11]). No diagonal dominant elements are systematically introduced, only some columns and rows are rescaled in $V_L V_R$ by the elements of the diagonal matrix D_R. We know of no theorem in numerical linear algebra where numerical behavior is improved by randomly scaling columns or rows, and therefore expect hardly any stabilization effect. This was also experienced by Loh *et al.*,[11] where the deficiency was cast rather moderately in the words: "Preliminary tests using Eqs. (5) and (7) suggest they help stabilize the simulation numerics but perhaps are not as robust as Eq. (3)".

In other words, only the computation of the Trotter-product was stabilized. In contrast, the inversion did not profit from the stabilization scheme, because immediately before the inversion, all scales are mixed again. The scheme in Eq. (A.4) must therefore be considered as unreliable for the computation of Greens functions at equal and nonequal times alike.

Appendix B. New Stabilization Scheme

B.1. *Equal time Greens functions*

We propose stabilize the Trotter-product by the QR-transformation after Householder with pivoting (QRHP), so that the entries of the diagonal Matrix D in Eq. (A.1) are ordered according to size. The resulting matrix R is no more trigonal, but trigonal dominant (i.e., the absolute value of the entries above the diagonal are larger than the absolute values of entries below) with benign condition number (of order 10 in our numerical experiments). In our test in Fig. A.1(a), the symmetry of the electron density if well preserved (in this case, up to more than eight digits). The use of the rank-revealing QR-decomposition[16] did not bring any significant improvements of accuracy compared to the QRHP in test runs.[10] As the rank-revealing QR-decomposition needs the output of the QRHP as input, we did not use this algorithm for production runs due to performance considerations.

B.2. *Nonequal time Greens functions*

It turns out that the algebraic formulation of the nonequal time Greens functions in Eqs. (5) and (6) can be used directly for a numerical stable implementation as long as $|G((k+1)\tau)| \leq |G(k\tau)|$ or $|G(-(k+1)\tau)| \leq |G(-k\tau)|$, respectively. After the equal time Greens function $G(0)$ has been stably computed, no further decomposition or stabilization is necessary, but the time-dependent Greens functions can be computed according to Eqs. (5) and (6). The $G((k+1)\tau)$ can be computed from the $G(k\tau)$ as long as

$$|G((k+1)\tau)| \leq |G(k\tau)|\,, \tag{B.1}$$

and the $G(-(k+1)\tau)$ can be computed from the $G(-k\tau)$ as long as

$$|G(-(k+1)\tau)| \leq |G(-k\tau)|\,. \tag{B.2}$$

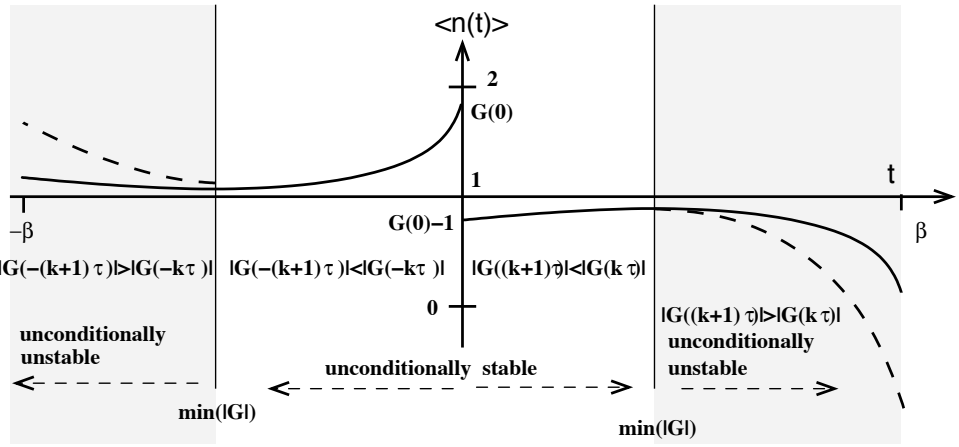


Fig. A.2. Sketch for the regions of stability and instability for the direct computation of the nonequal time Greens functions from the equal time Greens functions.

The Greens functions for all other imaginary times can be computed from the periodicity/antiperiodicity conditions for fermionic Greens functions, $G(t) = -G(t+\beta)$ and $G(t) = G(t+2\beta)$. As long as Eq. (B.1) or Eq. (B.2) is fulfilled, the condition for von Neumann stability is fulfilled, like in the ground state quantum Monte Carlo,[18] so no further stabilization is necessary. In Fig. A.2, we sketched the stable and unstable branches for the computation, which means that one branch must be computed from $\langle c_i(t)c_j^+(0)\rangle$, the other one from $\langle c_i^+(t)c_j(0)\rangle = \langle c_i(t)c_j^+(0)\rangle - \delta_{ij}$. For half-filling, the imaginary time point $t_{\min}$ where $|G(-(k+1)\tau)| \approx |G(-k\tau)|$ is at the imaginary time $t_{\min} = -k\tau \approx -\beta/2$. For fillings $n > 0.5$, the minimum norm is reached for $t_{\min} < \beta/2$, and due to the symmetry of the Greens function, for fillings $n < 0.5$, we will have $t_{\min} > \beta/2$. The point of the minimum norm of the Greens function fluctuates with the HS-configuration, so to minimize the errors, near $t_{\min}$ that branch (computation "from left" or "from right") must be chosen for which the condition Eq. (B.1) or Eq. (B.2) is fulfilled.

References

1. H.-G. Matuttis and N. Ito, *J. Phys. Soc. Jpn.* **70**, 401 (2001).
2. E. Y. Loh, J. E. Gubernatis, R. T. Scalettar, S. R. White, D. J. Scalapino and R. L. Sugar, *Phys. Rev. B* **41**, 9301 (1990).
3. G. Su, *Phys. Rev. Lett.* **86**, 3690 (2001).
4. G. Su and M. Suzuki, *Phys. Rev. B* **58**, 117 (1998).
5. J. E. Hirsch, *Phys. Rev. B* **31**, 4403 (1985).
6. M. Suzuki, *Comm. Math. Phys.* **51**, 183 (1976).
7. M. Suzuki, *Comm. Math. Phys.* **57**, 193 (1977).
8. M. Suzuki, S. Miyashita and A. Kuroda, *Prog. Theor. Phys.* **58**, 1377 (1977).
9. J. E. Hirsch, *Phys. Rev. B* **28**, 4049 (1983).
10. H.-G. Matuttis, *Determinanten Quanten Monte Carlo und Analytische Fortsetzung für das Hubbard Modell* PhD. thesis (Universität Regensburg, 1995).

11. E. Y. Loh, Jr., J. E. Gubernatis, D. J. Scalapino, R. L. Sugar, S. R. White and R. T. Scalettar, Stable matrix multiplication algorithms for low-temperature numerical simulations of fermions, *Interacting Electrons in Reduced Dimensions*, eds. D. Baeriswyl and D. K. Campbell, NATO ASI Series B, Vol. 213 (Plenum Press, 1989), p. 55.
12. M. Imada and N. Furukawa, *J. Phys. Soc. Jpn.* **60**, 810 (1991).
13. J. M. Singer, M. H. Pedersen, T. Schneider, H. Beck and H.-G. Matuttis, *Phys. Rev. B* **54**, 1286 (1996).
14. H.-G. Matuttis and N. Ito, Advances in the investigation of the minus sign problem for the fermionic case, *Computer Simulation Studies in Condensed-Matter Physics XIV*: *Recent Developments*, eds. D. P. Landau, S. P. Lewis and H. B. Schuettler (Springer, 2002) pp. 194–199.
15. D. J. Scalapino, *Phys. Rep.* **250**, 329 (1995).
16. T. F. Chan and P. C. Hansen, *SIAM J. Sci. Stat. Comput.* **13**, 727 (1992).
17. G. H. Golub and C. F. Van Loan, *Matrix Computations* (The Johns Hopkin University Press, 1989).
18. W. von der Linden, *Phys. Rep.* **220**, 53 (1992).