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NEGATIVE WEIGHTS IN QUANTUM MONTE CARLO SIMULATIONS AT FINITE-TEMPERATURES USING THE AUXILIARY FIELD METHOD

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We study the conditions under which negative weights (the sign problem) can exist in the finite-temperature, auxiliary field, quantum Monte Carlo algorithm of Blankenbecler, Scalapino, and Sugar. We specifically consider whether the sign problem arises from round-off error resulting from operations involving very ill-conditioned matrices or from topological defects in the auxiliary fields mirroring the space–time patterns of the physical fields. While we demonstrate these situations can generate negative weights, the results of our numerical tests suggest that these factors are most likely not the dominant sources of the problem. We also argue that the negative weights should not be considered as just a fermion problem. If it exists for the fermion problem, it will also exist for an analogous boson problem.

1. Introduction

With the explosive development of supercomputers over the past decade, there has been a parallel increase of interest to simulate the properties of systems of interacting electrons. The desire is not only to benchmark the approximate calculations of models that convey our understanding of the many novel states of matter but also to develop more accurate *ab initio* methods that will predict physical properties consistent with experimental measurements. The most significant impediment to performing these simulations, and thereby advancing our ability to do many-electron theoretical physics, is the "sign problem." Indeed, many proposed models of high temperature superconductivity remain incompletely tested because the sign problem is most severe in parameter ranges of experimental relevance.

The simulation algorithms are Monte Carlo-based and are devoted to finding either the zero temperature or the finite temperature properties of the systems. In the zero temperature algorithms, the sign problem is connected to the loss of "fermionic" character of the generated quantum mechanical wave function that is supposed to solve Schroedinger's equation.[1–3] The finite temperature algorithms

start with a quite different formalism but in most cases suffer a similar fate. These algorithms are almost always applied to simple, but still unsolvable, models of the electron interactions. These interactions, which are quartic functions of the electron operators, are removed from the problem by a "completing the square" operation[4] similar to

$$e^{A^4} = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} d\phi \, e^{-\phi^2 + 2\phi A^2} \tag{1}$$

where A is some operator and ϕ is an auxiliary Bosonic (scalar) variable. Next, the Gaussian integrals in the operator A are performed exactly, which converts the quantum problem of enumerating the electron configurations to one of enumerating the configurations of the auxiliary fields ϕ that occur with some weight w. This weight depends on all the ϕ fields (and the parameters of the model under consideration) and is used in Monte Carlo importance sampling of the auxiliary fields.

The objects of these finite-temperature simulations are estimates of thermodynamic averages of some physical observable B

$$\langle B \rangle_w = \frac{\sum_{\mathcal{C}} B(\mathcal{C}) w(\mathcal{C})}{\sum_{\mathcal{C}} w(\mathcal{C})} \tag{2}$$

where $\mathcal{C}$ represents a configuration of auxiliary fields and $w(\mathcal{C})$, its thermodynamic weight. In many cases, however, these configurations appear with a negative weight that in principle can be handled[5–7] by defining a "sign" s by $w = s|w|$ and re-expressing the average by

$$\langle B \rangle_w = \frac{\langle sB \rangle_{|w|}}{\langle s \rangle_{|w|}} \tag{3}$$

The "sign problem" refers to the empirical finding that the value of the average sign $\langle s \rangle_{|w|}$ approaches zero exponentially as the physical size of the system is increased and its temperature is decreased. This condition leads to infinite variance in the measured value.

The precise cause of the various sign problems in the above and related algorithms is a matter of active discussion while cures are sought. For the zero-temperature algorithms, like the ones mentioned above, the source of the sign problem is clearly the use of a Monte Carlo weight that has both positive and negative values. The situation for the finite-temperature algorithm is less clear.

Proposed cures to the sign-problem are often technical adjustments of the implementations of the algorithms that sometimes make the problem even worse! Recently, several zero-temperature algorithms without sign problems which are still the subject of research, have been proposed.[8,9] The finite-temperature methods have had less promising proposals for cures.[6,10–16]

In this paper, we will address the issues about the possible origin of the sign problem in the finite-temperature algorithm. To do so, we will consider, as in the seminal paper by Blankenbecler, Scalapino, and Sugar (BSS),[5] systems of spinless

fermions after the auxiliary fields have been introduced. Thus, our starting point is a Hamiltonian $H(\tau)$ for non-interacting electrons that are coupled linearly to external (auxiliary) fields which depends on imaginary-time τ. Averaging over these auxiliary fields restores the interactions, but weights of the interactions are sometimes as often negative as they are positive. We will be concerned with identifying conditions under which any given configuration of auxiliary fields is produced with a negative weight.

In Sec. 2, we summarize the approach of Blankenbecler *et al.*[5] A strength of their approach was the reduction of the problem to simply-constructed matrices with reasonably straight-forward matrix operations. Examining the properties of these matrices, we illustrate in Sec. 3 that while a sign problem is possible within the algorithm it is surprising that negative weights can be produced with such ease. In Sec. 4, we hypothesize that the sign problem is a consequence of round-off error or is symptomatic of non-perturbative mechanisms related to a topological defect in the auxiliary fields. We report results of numerical tests of these hypotheses and conclude these effects are not the dominant causes. Finally, in Sec. 5, we summarize our findings and make suggestions for additional research.

2. Algorithmic Summary

The starting point[5,17] is a path-integral formulation of a field theory in which the expectation value of an operator A is given by

$$\langle A\rangle = \int \mathrm{e}^{-S} A \Big/ \int \mathrm{e}^{-S} . \tag{4}$$

S is the Euclidean action defined at imaginary-time $\tau = it$, and the integrals are over all possible configurations of fields on which S and A depend.

We will be concerned with the continuum action

$$S = S_B + \int d\tau \int d^d x \psi^\dagger(x, \tau)\hat{O}\psi(x, \tau) \tag{5}$$

where S_B is the action associated with the auxiliary fields, $\psi(x, \tau)$ is the fermion field, and d is the number of space dimensions. $\hat{O}$ describes the fermion dynamics and contains the coupling to the auxiliary fields $\phi(x, \tau)$. Generally, $\hat{O}$ is of the form

$$\hat{O} = \frac{\partial}{\partial\tau} + H \tag{6}$$

and the fermion fields satisfy $\psi(x, \tau) = -\psi(x, \tau + \beta)$ where $0 \le \tau \le \beta = 1/kT$.

If the opeator A is independent of fermionic fields, then

$$\langle A\rangle = Z^{-1} \int \mathrm{e}^{-S_B} \det\left(\frac{\partial}{\partial\tau} + H\right) A \tag{7}$$

with

$$Z = \int \mathrm{e}^{-S_B} \det\left(\frac{\partial}{\partial\tau} + H\right) \tag{8}$$

The sign problem occurs when

$$D \equiv \det \hat{O} = \det\left(\frac{\partial}{\partial\tau} + H\right) \leq 0 \tag{9}$$

Blankenbecler *et al.*[5] show that

$$D = \det\left[I + \mathcal{T} \exp\left(-\int_0^\beta d\tau\, H(\tau)\right)\right] \tag{10}$$

where $\mathcal{T}$ is the time-ordering operator. With the discretization of the imaginary-time interval into L Trotter steps of length $\Delta\tau$, the matrix $\hat{O}$ becomes

$$\hat{O} = \begin{pmatrix} I & 0 & 0 & \cdots & 0 & B_1 \\ -B_2 & I & 0 & \cdots & 0 & 0 \\ 0 & -B_3 & I & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & I & 0 \\ 0 & 0 & 0 & \cdots & -B_l & I \end{pmatrix} \tag{11}$$

with I and B_m being $N^d \times N^d$ matrices where N is the number of lattice sites along each spatial dimension. The B_m are (or can be written as)

$$B_m = \mathrm{e}^{-\Delta\tau H_0/2} \mathrm{e}^{-\Delta\tau V_m} \mathrm{e}^{-\Delta\tau H_0/2}, \tag{12}$$

where H_0 is part of the Hamiltonian (often just the kinetic energy) that is independent of the auxiliary fields and V_m is the part that depends on the auxiliary fields (and everything else). This form for B_m is clearly Hermitian and can be shown to be positive-definite; therefore, B_m can be written as the exponential of some Hermitian matrix (effective Hamiltonian)

$$B_m = \exp[-\Delta\tau H_{\mathrm{eff}}(m\Delta\tau)] \tag{13}$$

By ***positive-definite***, we mean that

$$\langle x|B_m|x\rangle > 0 \tag{14}$$

for any non-zero state $|x\rangle$.[18]

For a given configuration of auxiliary fields, the inverse of $\hat{O}$ is the single-particle Green's function $\hat{G}_{m,m'}(l, l')$,[5,17] and it is easily shown that

$$D \equiv \det \hat{O} = \det(I + B_L B_{L-1} \cdots B - 1) \tag{15}$$

In a Monte Carlo calculation, the acceptance of one configuration of auxiliary fields relative to another depends on the ratio of D for the two different configurations. In many applications, where the interaction is very local (as in the Hubbard

model), this ratio at imaginary-time step m reduces to a simple expression involving $1 - \hat{G}_{m,m}(l, l)$

$$D'/D = 1 + [1 - G_{m,m}(l, l)][e^{-\Delta\tau\Delta V_m(l)} - 1] \tag{16}$$

where $\Delta V_m(l)$ is the change in the potential in state l at time m caused by the change in the configuration of auxiliary fields. When $1 - \hat{G}_{m,m}(l, l)$ is less than 0 or greater than 1, the ratio can become negative and, depending on the value of $\Delta V_m(l)$, a sign problem can occur. In the convention of BSS,[5] one minus the equal-state, equal-time Green's function is the expected electron occupancy for the state. Furthermore, this Green's function is the exact Green's function (within the error caused by the Trotter approximation) for the given configuration of auxiliary fields. Thus, a sign problem can only occur when the Pauli exclusion principle has been violated. Just as significantly, such non-physical behavior can occur without there being a sign problem!

We will first address only the issues concerning the sign of D. Then, we will focus on the appearance of the non-physical behavior. Since the value of a determinant of a matrix is the product of the eigenvalues of the matrix, we will start by discussing expected properties of the eigenvalues of the matrices $\hat{O}$ and P where

$$P = I + B_L B_{L-1} \cdots B_1 \tag{17}$$

3. Matrix Properties

3.1. *General considerations*

We start by asking the question: "Within the BSS formalism, independent of specifics of a numerical implementation, can a sign problem occur?" In particular, we will first investigate whether one can ever have

$$D \leq 0\,. \tag{18}$$

We will be able to make limited general statements, but we do find that the structure of $\hat{O}$ allows us to derive some bounds on its eigenvalue spectrum.

First, we will define the matrix M to be $B_L B_{L-1} \cdots B_1$. Since the B matrices are positive-definite and M is formed by a product of the B matrices, $\det M > 0$. The product of two different Hermitian matrices, however, is, in general, not Hermitian, so M is, in general, not Hermitian. The loss of Hermiticity means the eigenvalues of M need not be real. By a similarity transformation, we can put M into triangular form where the diagonal elements μ_i are its eigenvalues. Accordingly, $\det M = \prod_i \mu_i > 0$. The condition $\det M > 0$ assures that we have a complete set of eigenvectors, but these vectors are in general not mutually orthogonal. Thus, we can write

$$\det(I + M) = \prod_i (1 + \mu_i) \tag{19}$$

and be tempted to write

$$\det(I + M) = \prod_i (1 + e^{-\beta m_i}) \tag{20}$$

to develop the appearance of the Fermi–Dirac partition function to which the weight should reduce. If M were Hermitian this would be a useful step, but the lost of the Hermiticity of M means that the μ_i need not be real, and even if they are real, the absence of positive-definiteness means that some can be negative. If some are negative, then there must be an even number of them to avoid the sign problem. For the negative eigenvalues, one would be tempted to write

$$1 + \mu_i = 1 - e^{-\beta m_i} \tag{21}$$

which appears bosonic, but since the eigenstates are not orthogonal, the physical interpretation of this result is unclear. The non-positive definiteness was noted by Blankenbecler *et al.*, but they believed that a sign problem was unlikely.[5]

To understand the eigenvalue spectrum a bit more, we rewrite $\hat{O}$ as $\hat{I} - \hat{N}$ where

$$\hat{N} = \begin{pmatrix} 0 & 0 & 0 & \cdots & 0 & -B_1 \\ B_2 & 0 & 0 & \cdots & 0 & 0 \\ 0 & B_3 & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & 0 & \cdots & B_L & 0 \end{pmatrix} \tag{22}$$

The eigenvalues η of $\hat{N}$ satisfy

$$\det(\eta\hat{I} - \hat{N}) = \det(\eta^L I - B_l B_{L-1} \cdots B_1) = \det(\mu I - M) = 0 \tag{23}$$

Consequently, $\eta^l = \mu$, which means the eigenvalues of $\hat{N}$ are L-fold degenerate and completely determined by the eigenvalues of M.

3.2. *Specific considerations*

To make additional general statements about the eigenvalue spectrum of M without additional information about M appears difficult, but clearly the general structure of the BSS algorithm admits the possibility of negative weights. For the models most commonly simulated by this algorithm, the Anderson and Hubbard models, we can say that in a Wannier basis M is a *positive* matrix. By this we mean

$$\langle x|M|y\rangle > 0 \tag{24}$$

where $|x\rangle$ and $|y\rangle$ are any two Wannier states. We argue as follows: In the simulations of these models, H_0 is typically the kinetic (hopping) energy, which in a

Wannier basis has some negative off-diagonal elements (connecting sites between which hopping is allowed) with all other elements being zero (connecting states between which hopping is not allowed). The remainder of the Hamiltonian can be lumped into V_m and is diagonal in this basis. The validity of the algorithm requires $\Delta\tau$ to be small so we can write $\exp(-\Delta\tau H_0) \approx I - \Delta\tau H_0$ which in a Wannier basis will consist only of positive and zero elements. (Actual numerical construction of this exponential supports this conclusion.) The exponential of V_m is a positive-definite diagonal matrix in the Wannier basis, and hence has only non-negative elements. The product of two matrices whose elements are non-negative can only produce a result whose elements are non-negative. The result of a product of a large number of such matrices is a matrix whose elements are all positive. We represent this condition as $M > 0$. In contrast, the least that positive-definiteness implies is that the diagonal elements must be positive in ***any*** basis. Although it is difficult to see how general this property is, it being true for the Hubbard and Anderson models — for which the sign problem exists and is severe — warrants consideration of what in general can be said about the eigenvalue spectrum of such matrices.

Perron proved that a positive matrix has as its largest eigenvalue a positive number and the moduli of all other eigenvalues must be less than this number.[19] The implication of this theorem is all the eigenvalues of M must then lie in a circle of radius r centered at the origin of the complex plane. (As $\Delta\tau \to 0$, one expects r to approach the lowest eigenstate of $\exp[-\beta H(\tau)]$.) Accordingly, by Gerschgorin's theorem,[20] the eigenvalues of $I+M$ lie in a circle of radius r centered at the value of 1 on the real axis. Thus, if $r < 1$, there is no sign problem. Because the eigenvalues of $\hat{O}$ are the Lth root of $I+M$, these bounds mean that the eigenvalues of $\hat{O}$ lie in a circle of radius $r^{1/L}$ centered at 1. As L becomes large for a fixed value of β, which is required for the validity of the BSS algorithm, this radius approaches unity. In particular, if $r > 1$, the bounding region for the eigenvalues begins to exclude the left-half complex plane and it would seem less likely to have a sign problem.

4. Negative Weights

Although the eigenvalue spectrum of M and $\hat{N}$ are connected, the spectra have quite differently sized bounding regions. This difference suggests that these matrices are very differently conditioned. If W is the bandwidth of $H(\tau)$, the condition number of M is roughly $\exp(\beta W)$, while for $\hat{N}$ it is $\exp(\Delta\tau W) \approx 1 + \Delta\tau W$. M is known to be very ill-conditioned, and at low temperatures extraordinary measures are required just to construct it accurately.[17,21,22] Even more difficult is computing $(I+M)^{-1}$ and cyclic variants $(I + B_m \cdots B_1 B_L \cdots B_{m-1})^{-1}$, which are equal-time components of the single-particle Green's function. The matrix $I + M$, with its cyclic variants, are used in the simulations because the order of these matrices is a factor of L less than the order of $\hat{O}$, and the necessary matrix operations in the algorithm scale as the order cubed. Because of the ill-conditioned nature of these matrices, it is natural to ask whether the sign problem is a numerical consequence of the ill-conditioning.

So far, we have considered only an arbitrary unspecified configuration of auxiliary fields. In some cases, the topology of these fields is directly connected with the topology of the actual fermion fields. For example, for the discrete auxiliary fields, Hirsch[23] showed that the spin–spin correlation function was directly related to the thermodynamic average of the correlation of the auxiliary fields on different sites. Although the auxiliary fields do not map directly onto all possible physical correlation functions, patterns in these fields can be reasonably expected to be connected with the physical state being simulated. As the temperature is lowered, distinct electronic or spin phases in the physical problem usually develop. Is it possible, even though the left-hand complex plane represents only a small portion of the admissible eigenvalue spectrum, that the physical requirements of the model being simulated tend to produce configurations of auxiliary field associated with these regions?

These numerical and topological considerations represent two possibilities for the sign problem that can be investigated by numerical experiment. The sign problem could occur for both reasons. Other reasons are not necessarily excluded.

4.1. *Numerical considerations*

Our numerical tests were all performed on a 4 × 4 Hubbard model at a variety of values of the interaction U and electron fillings. Instead of a Hubbard–Stratonovich transformation with a Gaussian-distributed field that in principle can assume any value between plus and minus infinity, we used the discrete transformation of Hirsch[23] with an Ising-like field that has only two finite values. This transformation is commonly used in lattice fermion simulations because it equilibriates and produces decorrelated measurements more rapidly than a simulation using the continuous field.[24] In the present case, the important property of this transformation is that it produces an interaction V that is bounded. In the case of the continuous field transformation, the interaction, in a practical sense, is bounded, but the Hubbard–Stratonvich fields can assume values such that the exponential of V produces a matrix whose elements span many orders or magnitude. Such a situation itself can generate severe numerical problems. We chose to avoid this situation. Additionally, since the Hubbard model describes electrons with spin, the problem has an up and down spin determinant. We, for convenience, examined only one spin.

In our tests, we made no effort to equilibriate the system. Instead, we would generate a random distribution of Hubbard–Stratonvich fields, produce the matrix $\hat{O}$, and calculate its inverse $\hat{G}$. Then, we computed several figures of merit: The number of diagonal elements of $\hat{I} - \hat{G}$ less than 0 or greater than 1, the maximum and minimum values of the elements of $\hat{G}$, the norm of the residual matrix, the norm of the error matrix, and the condition number of $\hat{O}$. Since for a given configuration of Hubbard–Stratonvich fields, the diagonal elements of $\hat{I} - \hat{G}$ are electron occupancies, values less than 0 or greater than 1 are unphysical. The occurrence of

such unphysical values does not necessarily mean that a sign problem has occurred. We recall the sign problem requires positive values of the occupancy well in excess of unity.

For a fermion problem, it perhaps seems reasonable that the elements of the Green's function $\hat{G}$ would have elements whose absolute value is bounded, perhaps even by the value of 1. Although we have been unable to prove such bounds, monitoring the maximum and minimum elements of $\hat{G}$ provided some insight about what was happening. As a block matrix in imaginary-time, $\hat{G}$ is antisymmetric in the unequal-time blocks. The maximum and minimum elements of $\hat{G}$ are simple signals of whether this anti-symmetry is present. When we felt that we had successfully inverted the matrix, we found that the minimum and maximum, within numerical error were equal in magnitude but opposite in sign.

The residual matrix $\hat{R}$ is defined by

$$\hat{O}\hat{G} - \hat{I} = \hat{R} \tag{25}$$

while the error matrix $\hat{E}$ satisfies

$$\hat{O}\hat{E} = \hat{R}. \tag{26}$$

To quantify the "size" of a matrix, we used the L_1-matrix-norm[18] which for any matrix A with elements a_{ij} is

$$\|A\| = \max_j \sum_i |a_{ij}|. \tag{27}$$

The size of the residual and error provides measures of the accuracy of the inverse, but these measures, when finite precision arithmetic is used, are incomplete unless accompanied by an estimate of the condition number of the matrix being inverted. This number κ for a matrix A is defined by

$$\kappa = \|A\| \ \|A^{-1}\|. \tag{28}$$

If the arithmetic is done to a precision represented by 10^{-t} and $\kappa = 10^d$, the precision of the result of the matrix inversion is expected to be no better than 10^{d-t}.[18] For 32 and 64 bit arithmetic, t is about 7 and 15. The norm of $\hat{O}$ is generally reasonably sized, 10^0 to 10^2. On the other hand, the norm of $\hat{G}$ is generally orders of magnitude larger. With 32 bit arithmetic, it is easy to lose all precision in the inverse.

We tried four methods to compute the inverse: A sparse matrix method,[25] the method of modification,[26] Gaussian elimination with partial pivoting,[27] and Gaussian elimination with complete pivoting.[18] We judged these methods to be nearly equally effective. They gave the same result unless total precision was on the verge of being lost, in which case the sparse matrix method was the least stable.

The sparse matrix method, however, required an order of magnitude less computer storage and computer time than the other three and evolved into the method used the most.

We computed the inverse for a number of different values of U (0 to 8) and electron filling (0 to 2) for various values of fixed β (1 to 30) with different values of $\Delta\tau$ (0.1 to 0.5) and for various values of fixed $\Delta\tau$ for different β. As we lowered the temperature, a general feature was the growth of the unequal time elements of $\hat{G}$ to magnitudes of 10 to 10000 before the appearance on unphysical behavior in the diagonal elements.

Using 32 bit arithmetic, we found non-physical behavior developed as $\hat{O}$ was becoming ill-conditioned with respect to inversion at that level of precision. Computing the inverse using 64 bit arithmetic and the same configuration of Hubbard–Stratonvich fields did not remove the non-physical behavior. While ill-conditioned with respect to inversion with 32 bit arithmetic, the matrix was reasonably well-conditioned for inversion with respect to 64 bit arithmetic. Although non-physical behavior can be produced by round-off error, in general, we could eliminate this concern but could not in general eliminate the non-physical behavior.

Once the non-physical behavior appeared, the number of non-physical values would change, and sometimes disappear, as different configurations were generated. Changing the value of U and $\Delta\tau$ reasonably had less of an effect on non-physical behavior then did lowering the temperature. A surprising result was that the half-filled case behaved worse than all other fillings, even though it was not the most ill-conditioned case. In actual simulations, it is the product of the up and down spin determinants that are monitored for a negative value. In the half-filled case, these determinants must be of the same sign; hence, the half-filled case has no sign problem. Clearly, the absence of the sign problem does not guarantee physical behavior in the simulation.

An interesting case was the one for $U = 0$. Here, there are no Hubbard–Stratonovich fields and no Trotter approximation. We can also calculate the Green's function from the eigenvalues and eigenvectors of the non-interacting problem and compare the result with the one obtained by the matrix inversion procedures. Using 32 bit arithmetic, we found excellent agreement between these methods down to 50, the lowest β used, with as few as 10 Trotter steps. Using the stabilized methods to invert $I+M$, with a $\Delta\tau = 0.25$ (a standard value), we found that the inversion with 32 bit arithmetic became unstable around $\beta = 5$. This instability was the reason why the stabilized method was excluded from most of our tests.

Our tests cast doubts on, but do not rule out, the possibility of the non-physical behavior or the sign problem being primarily caused by round-off error due to the handling of ill-conditioned matrices. What have shown is that we can accurately invert the matrix. If the precision of the matrix elements is much lower the machine precision 10^{-t}, then it is possible that the ill-conditioning will still produce a result for the inverse that lacks any meaningful precision. (This is another way of expressing the computational maxim, "Garbage in. Garbage out.") The

precision of the result will not be controlled by the hardware but by the accuracy of the matrix elements of $\hat{O}$. The accuracy of these elements depends on the Trotter approximation. Are we approximating $\exp[\Delta\tau(H_0 + H_1)]$ accurately enough?

We performed some tests comparing the difference in computing $\exp[\Delta\tau(H_0 + H_1)]$ by $\exp \Delta\tau H_0 \exp \Delta\tau H_1$, by $\exp \Delta\tau H_1 \exp \Delta\tau H_0$, or by $\exp(\Delta\tau H_0/2)\times \exp \Delta\tau H_1 \exp(\Delta\tau H_0/2)$. We found that to reduce the norm of the differences between these various approximations to 1% or less required a $\Delta\tau$ of 0.01 or less, which is a factor of 10 to 50 smaller than the value of $\Delta\tau$ normally used. Using a $\Delta\tau$ this small for a value of β at which the non-physical behavior occurs makes the order of the matrix $\hat{O}$ extremely large and its inversion would require computing time and storage one to two orders of magnitude more than we are currently using. Accordingly, we were unable to investigate this issue at this time.

One can also wonder whether the non-physical behavior we are seeing is linked to the fact that the Hubbard–Statonovich fields we are using are inconsistent with the configuration of fields appropriate to the temperatures we specified. This is another possibility that would require considerable computing time to investigate. This investigation too was postponed until another time. What we will now discuss are the results of another investigation concerned with the question of whether specific physical properties of the Hubbard–Stratonvich fields produce the non-physical behavior.

4.2. *Topological considerations*

Although we know the determinant is never a complex number, it is instructive, however, to write the effective action for the auxiliary fields ϕ in a general form,

$$\det \hat{O}(\phi) = \exp[i\pi n(\phi) - S(\phi)] \tag{29}$$

where n is an integer function of the auxiliary field $S(\phi)$. From the work of Su, Schrieffer, and Heeger,[29] and others,[30] we know that n is the degeneracy of zero modes of the matrix of which we are taking the determinant. Here, for illustrative purposes, we show why this is so: Using the operator identity,

$$\log \hat{O} = \log(\hat{I} - \hat{N}) = \int_0^1 dy \frac{1}{\hat{I} - y\hat{N}} \tag{30}$$

we write the determinant as

$$\det \hat{O} = \exp[\mathrm{Tr} \log \hat{O}] = \exp\left[\mathrm{Tr} \int_0^1 dy \frac{1}{\hat{I} - y\hat{N}}\right] \tag{31}$$

If we denote N_i as the eigenvalues of $\hat{N}$, then the exponential becomes a summation of integrals, $\sum_i \int_0^1 dy \frac{1}{1-yN_i}$. Since the integrand can be divergent, the integration is separated into a principal and an imaginary part,

$$\frac{1}{1 - y\hat{N}_i} = P\frac{1}{1 - y\hat{N}_i} + i\pi\delta(1 - y\hat{N}_i) \tag{32}$$

Therefore, whenever N_i is real and greater than one, an $i\pi$ contribution to the argument of the exponential occurs. An odd number of such contributions will render the determinent negative.

These zero modes are topological solitons. To see the type of auxiliary fields that create these zero modes, we take the continuum limit and study the operator,

$$\hat{O} = \partial_\tau - \partial_x^2 + \omega^2 + \lambda\phi(x, \tau) \tag{33}$$

where ∂_x^2 is continuum limit of lattice hopping, and ω^2 is the chemical potential. We can always adjust the chemical potential so that the zero modes are obtained from $\hat{O}\xi = 0$, where ξ satisfy the boundary condition, $\xi(x, -\beta/2) = -\xi(x, \beta/2)$. Since the operator $\hat{O}$ is real, we are only interested in a real solution, because for any complex solution ξ, its complex conjugate ξ^* is also a solution and hence the product of the eigenvalues, which is the determinant, is always positive.

The simplest case is when $\phi(x, \tau)$ is independent of x. Then, there is no real solution. In general, for a given $\phi(x, \tau)$, deciding if the differential operator has a real solution is difficult, so we obtain the solution by construction. For a system with finite size L, we let the temperature be low enough so that $v\beta \gg L$, here v is an arbitrary parameter determined by the energy of the soliton or the initial condition. Then $\xi = \mathrm{sech}(v\tau - x)$ satisfies the boundary condition and is a zero mode solution, provided that the auxiliary field is such that $\lambda\phi(x, \tau) = \mathrm{sech}^2(v\tau - x) - v\tanh(v\tau - x) + \omega^2$. This solution is reminiscent of the Su-Schrieffer–Heeger soliton solution, but here, space is not limited to one dimension. For spacial dimensions higher than one, the soliton of this type is unstable, but the zero mode effect is still there. The instability simply implies that this solution cannot be a ground state solution.

The auxiliary field of the above soliton type can certainly be achieved during the course of a simulation. The question is whether this is the configuration that prevails. If the system under study is the Hubbard model and the auxiliary field decouples the magnetic sector, then adding a staggered field, i.e., $\xi(x, \tau) = (-)^x\xi_0(x, \tau)$, to the above solution and changing the auxiliary fields accordingly makes the soliton configuration a very probable configuration, if not the most probable one, in the simulation at close to half-filling. The reason is simple: First, it can be shown straightforwardly that

$$\langle\phi(x, \tau)\phi(x', \tau')\rangle \propto \langle m_z(x, \tau)m_z(x', \tau')\rangle \tag{34}$$

where m_z is the magnetization along z-direction. Secondly, at half-filling, antiferromagnetic order with staggered magnetizations does exist.[28] Away from the half-filling, the order is destroyed by the creation of domain walls randomly distributed in time and space. These walls are solitons.

Numerical realization of these soliton configurations is, in principle, simple. One prescription is to generate a perfect anti-ferromagnetic order uniform along the imaginary time axis, then flip several spins to form a wall, and then move the position of the wall along the imaginary time axis. The problem with this presciption,

as with others, is that no guarantee exists that negative weights will be generated. The apparent difficulty is that there are differences between a soliton on a lattice and a soliton in the continuum. Especially along the imaginary time axis, where for a given $\Delta\tau$, one can in principle insert as many additional time slices as one wishes, and depending on the configuration inserted, one may change the topology. In other words, the winding number is not well defined. This freedom exists on a lattice but not in the continuum.

5. Concluding Remarks

We comment that although the spin problem manifests itself in the breakdown of the fermionic character of the system under investigation, it should not be regarded exclusively as a fermion problem.

We first observe that we can rewrite the fermionic determinant by a product of two bosonic ones,

$$\det(I + M) = \frac{\det(I - M^2)}{\det(I - M)} \tag{35}$$

We can regard $\det(I - M)$ and $\det(I - M^2)$ as bosonic partition functions because for a Boson field problem with the same action matrix

$$\frac{1}{\det(I - M)} = \int \exp\left[\int d\tau \int d^d x \psi^*(x, \tau)\hat{O}(x, \tau)\psi(x, \tau)\right] \tag{36}$$

where $\psi(x, \tau)$ is now a Bosonic field. This means that whenever the minus sign occurs in the fermionic determinant, the two bosonic partition functions must differ in sign; therefore, one of them must be negative.

If we expand the bosonic determinant term by term through the fugacity expansion, i.e., by terms representing 0 particles, 1 particle, etc., we find

$$\frac{1}{\det(I - M)} = I + \operatorname{Tr} M + \frac{1}{2}[(\operatorname{Tr} M)^2 + \operatorname{Tr} M^2] + \cdots \tag{37}$$

This relationship easily follows if one multiplies the matrix M by a variable y, expands the inverse determinent of $I - yM$ in powers of y,

$$\begin{aligned}\frac{1}{\det(I - yM)} &= \prod_i \frac{1}{1 - y\mu_i} \\ &= \sum_{k_1, k_2, \ldots, k_N} \mu_1^{k_1}\mu_2^{k_2}\cdots\mu_N^{k_N} y^{k_1 + k_2 + \cdots + k_N}\end{aligned} \tag{38}$$

and then compares the coefficients of the same power of y.

We now argue that every term in the above expansion or in the expansion of $\det(I - M^2)^{-1}$, is positive because $\operatorname{Tr} M$ is positive since $M > 0$ (at least for models

of major interest). Thus, we have a dilemma. The positivity of Tr M implies there is no sign problem whereas for the major models a severe sign problem in fact exists.

A careful examination of the sum suggests it might be divergent for certain auxiliary field configurations. The situation is probably similar to

$$-1 = \frac{1}{1-2} = 1 + 2 + 2^2 + 2^3 + \cdots + 2^k + \cdots \tag{39}$$

The actual situation is difficult to express analytically.

A divergent series can be viewed as another example of the zero mode we have discussed in the previous section. Since those solitons are unstable in $(2+1)$-dimensions, it is unlikely that they contribute significantly to the ground-state properties of the model. During the course of simulation, however, these solitons have to be created in order to access to the true ground state configuration. If the true ground state is non-degenerate, one should be able to equilibriate the system first with the presence of large number of minus signs, and as the ground state is approached, the value of the average sign will drastically decrease towards zero and eventually stabilize to positive value. From our experience with the Hubbard model, this scenario is not the case, especially in the region close to half-filling. We believe that this situation is connected with the ground state being degenerate when the finite lattice energy shell is not completely filled.[22] When the energy shell is incompletely filled, then different ways of drawing the Fermi surface exist and thus the ground state is degenerate. In fact, if one considers the change in the shape of Fermi surface as an excitation of the Fermi liquid, then in the degenerate case, those excitations have zero energy. For very large lattice size, say 30×30, the sign problem caused from these zero modes should be reduced because a filled energy shell exists at approximately 0.90 filling.

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