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COMPUTER SIMULATION FOR INTERACTING FERMIONS: A NOVEL TECHNIQUE BASED ON THE HUBBARD STRATONOVICH TRANSFORMNATION

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INTRODUCTION

The many-body problem of interacting quantum particles has been a subject of interest for many years. Unfortunately very few models which take the correlation into consideration are exactly solvable ones (1D Hubbard chain and its continuous limit: the δ-function gas for particles in a continuum). Therefore several approximate techniques have been used to treat correlation for systems of physical interest. Among this methods it is worth mentioning the Configuration Interaction CI (which is limited to very few electrons) , the many body perturbation theory (Hartree, Hartree-Fock) and the Local Density Approximation –LDA–. However these methods have two important drawbacks: either they are not systematically convergent to the exact solution, even in case an infinite computation time would be available, or they require a prohibitive amount of computer time. As an example in the full CI method the computation costs grows exponentially as the number of electrons in the molecule increases. Current approximation methods have costs ranging from the third power to the seventh power of the number of electrons. On the other hand binding energies are only a tiny fraction of total molecular energies. This makes high precision vital creating extreme difficulties in justifying the wholesale simplifications needed to reduce computational costs further.

Recently there has been progress,which looks very promising, in the simulation of quantum systems, using The so called Quantum Monte Carlo method (QMC). The goal of this method (Ceperley 1981, Ceperley and Alder 1984, Kalos 1984) is to obtain the exact ground state properties of a many body system by numerically solving the Scrhodinger equation. The imaginary time evolution $|\psi_G >= e^{-\hat{H}t}|\psi_0 >$ of any initial state $|\psi_0 >$ is proportional after infinite time to the exact ground state of the hamiltonian $\hat{H}$ because the operator $e^{-\hat{H}t}$ filters only the ground state component of $|\psi_0 >$ with the same simmetry property. In practice this is achieved by means of iterative algorithms, which propagate the wave function from a suitable starting guess to the exact ground state value. Thus in the Diffusion Monte Carlo method one is concerned directly with the evolution in imaginary time of the wave function, which corresponds to a diffusion process in configuration space. In the Green's Functions Monte Carlo, on the other hand, a time integrated form of the Green's function or resolvent is used to propagate the wave function. Even though the latter methods have been shown to be very promising for boson systems, there are still heavy problems when the methods are applied to fermions. The main difficulty arises from the antisimmetry of the fermion wave function. In fact the mentioned diffusion

evolution in configuration space can be applied only to positive definite objects that can be considered as density distributions. In this way the fermionic wave function, which due to its antisimmetry has positive and negative values, must be decomposed into the difference of two density distributions. Each one evolves with a diffusion process but the antisimmetry of the wave function cannot be independently verified by each of the two positive component. Then each density distribution has a small projection to the more stable boson ground state. This clearly produce a numerical instability for long time evolution.

New possibilities of approaching the many body electronic problem are discussed in the present thesis using a well known method: the Hubbard-Stratonovich Transformation (HST). This transformation has been known for long time in many branches of physics but only very recently it has been used in computer physics (Koonin et al., Blankenbecker et al. 1981, Hirsch and Scalapino 1986).

The imaginary time evolution $e^{-\hat{H}t}$ is numerically tractable when the Hamiltonian contains only one body operators and no interaction term. The HST is basically a method that allows to transform a many-body operator as a coherent superposition of one-body operators. In this way the HST transforms the many body problem in a functional integral over variables σ. This functional integration is performed by evaluating the propagation of a test function $|\psi_0>$ in a time dependent one body hamiltonian containing the integration variables σ. As far as the functional integral is concerned, it is calculated using a statistical method which is well established in literature: the Langevin dynamic. Our method is similar to QMC, as far the imaginary time evolution of a trial wave function is concerned, but at difference of the QMC it has the considerable advantage to preserve the antisymmetric property of the fermion wave-function at any time of such evolution. In the present thesis we also show how to preserve such property in a very efficient numerical way (see ch. 4).

Until now the most successful application of the HST was done by Hirsch and Scalapino (Blankenbecker and al. 1981, Hirsch and Scalapino 1986, Hirsch 1985), using a discretized version of the HST in which the functional integration is replaced with a trace over Ising variables (σ assumes the values $+1$ or -1). The goal of their calculation is to evaluate the finite-temperature partition function of a short range interacting system of electrons. However the discretized version of the HST can be used only for such short range interaction and has therefore a limited applicability. Moreover this method shows to be unstable for very low temperatures, while numerical tests confirm that our method can reach the $0°K$ limit without showing any instability.

Our method allows to investigate the $0°K$ properties of a many-body quantum system

described by a real (unfortunately the complex case is not clear yet) Hamiltonian $\hat{H}$ acting onto a finite Hilbert space of dimension D (computer can only deal with finite systems) in which an HST can be performed. All the usual electronic Hamiltonians (in solid state physics) which do not contain the magnetic field belong to this class. In order to check the reliability of this new method, I will apply this method to a very simple model belonging to the mentioned class of Hamiltonians: the $1D$ Hubbard model with periodic boundary conditions. However it should be kept in mind that the most important advantage of the present method is its generality:

1) it can be used for bosons as well as fermions (!);

2) it can be used for short ranged interactions as well as long range interactions;

3) as it can be found in the following the present method is numerically stable and it is systematic. In fact we give a mathematical argument which states the convergence of the method under reasonable hypothesis (see ch.3).

From this point of view the method has a big advantage compared with the QMC, where a numerical simulation is possible only with a very good initial guess of the ground state wavefunction.

Numerical tests, using our novel technique, shows the reliability of the results even using non-optimal trial function $|\psi_0>$.

As any statistical method the computer time required for its practical use is still close to the "limits" of the technological possibilities for system size of interesting application. Hopefully the increasing powerful of computers and the application of HST will make possible the numerical solution of the electronic structure problem in the same footing of a simple numerical integration.

CHAPTER I

A functional integral formulation for interacting fermions:

the Hubbard-Stratonovich transformation

As we have already mentioned in the introduction the ground state $|\psi_G>$ of a many body system can be written in the following formal way :

$$|\psi_G> = \lim_{t\to\infty} \frac{e^{-\hat{H}t}\,|\psi_0>}{||\, e^{-\hat{H}t}\,|\psi_0>\,||} \tag{1.1}$$

where as usual the symbol $||\ |\psi>||$ indicates the L_2 norm of an arbitrary vector $|\psi>$, and from now on we will call $|\psi_0>$ in expression (1.1): the trial wave function. In fact the (imaginary) time evolution in (1.1) of an arbitrary trial wave function is easily obtained from its expansion in terms of the eigen functions $|\psi_i>$ of the Hamiltonian H as:

$$|\psi(t)> = \frac{\sum_i N_i\, e^{-E_i t}\,|\psi_i>}{||\sum_i N_i\, e^{-E_i t}\,|\psi_i>\,||}, \tag{1.2}$$

here E_i is the energy eigenvalue corresponding to $|\psi_i>$ and the coefficients N_i are fixed by the initial condition, i.e. by the chosen trial wave function: $N_i = <\psi_0\,|\,\psi_i>$. Clearly for long time (1.1) is verified, provided $N_0 \neq 0$, with an error which is exponentially decreasing like:

$$e^{-E_{gap}t} \tag{1.3}$$

where $E_{gap} = E_1 - E_0$ is the gap between the first excited energy and the ground state energy. Thus the problem of determining the ground state eigen-function of an Hamiltonian $\hat{H}$ is equivalent to that of solving eq.(1.1).

The evaluation of the propagator (1.7) is numerically (Fest et al. 1982, Nobile and Roberto 1986) tractable when the Hamiltonian $\hat{H}$ contains only one body operators. In order to overcome the latter difficulty it is worth mentioning that a very simple relation allows to write a many-body operator

$$e^{\alpha^2\hat{O}^2} \tag{1.4}$$

by means of an integral containing only one-body hermitian operators $\hat{O}$:

$$e^{\alpha^2\hat{O}^2} = \frac{\int_{-\infty}^{+\infty} d\sigma\, e^{-\alpha\sigma\,\hat{O}-\frac{1}{2}\sigma^2}}{\int_{-\infty}^{+\infty} d\sigma\, e^{-\frac{1}{2}\sigma^2}}. \tag{1.5}$$

The last relation can be very easily verified by expanding the R.H.S. of the previous equation in powers of $\hat{O}$ and using the trivial gaussian averages

$$<\sigma^{2k}> = \frac{(2k)!}{k!} \tag{1.6}$$

Equation (1.5) is very instructive and represents the fundamental step in the HST because it allows to write a many body operator as a coherent superposition of single particle operators. This step, as we shall see in the following, allows to write the propagator (1.1) in a numerical feasible form. As is also clear the previous transformation (1.5) can be applied only for negative definite two-body operators contained in the hamiltonian $\hat{H}$ unless considering imaginary α. While this property is certainly not true in general, it can always be guaranteed to be so, as shown in app.1, for quite general two-body fermionic operators.

However the problem of calculating

$$e^{-\hat{H}t} \tag{1.7}$$

is not completely solved yet. In fact a general hamiltonian is usually the sum of a kinetic operator $\hat{T}$ and a two body term $\hat{V}$.The problem in fact derives from the non-commutativity of $\hat{V}$ and $\hat{T}$. Hence

$$e^{-(\hat{T}+\hat{V})t} = e^{-\hat{T}t}\, e^{-\hat{V}t} \tag{1.8}$$

is not verified in such a case. On the other hand for infinitesimal propagation $t = \Delta T$ in eq.(1.8) the effect of the commutator can be neglected up to $o(\Delta T^2)$ and for a better accuracy:

$$e^{-\hat{H}\Delta T} = e^{-\frac{\Delta T}{2}\hat{T}}\, e^{-V\Delta T}\, e^{-\frac{\Delta T}{2}\hat{T}} + o(\Delta T^3) \tag{1.9}$$

Therefore, noting that $e^{-\hat{H}t}$ can be formally written:

$$e^{-\hat{H}t} = \prod_{i=1}^{N_T} e^{-\hat{H}\Delta T} \qquad where\, \Delta T = \frac{t}{N_T} \tag{1.10}$$

we have in general all the ingredients to write the full many-body propagator in terms of a coherent superposition of single particle ones: a more convenient form from the numerical point of view.

In the present thesis we shall apply in detail the mentioned strategy to a model which is simple enough, so that we can compare the numerical results with exact analytic one, but still so interesting to contain all the difficulties for the computer simulation of interacting fermions.

A realistic model which takes the correlation into consideration and which is exactly solvable in one-dimension is the short range one-band model considered by a number of authors (Takahashi 1969, Ovchinnikov 1970, Soos and Ramasesha 1984, Anderson, Lieb and Wu 1968, Shiba and Pincus 1972, Yokoyama and Shiba 1987, Takahashi 1977). In this model one pictures the electrons in a narrow energy band hopping between the localized states of neighboring lattice sites with a repulsive interaction energy between two electrons of opposite spins occupying the same lattice site.

Consider a crystal (one, two, or three-dimensional) of N_a lattice sites with a total of $N \leq 2N_a$ electrons. It is supposed that the electrons can hop between the Wannier states of neighboring lattice sites, and that each site is capable of accommodating two electrons of opposite spins, with an interaction energy $U > 0$. The Hamiltonian to consider is then:

$$\hat{H} = T \sum_{<i,j>,\sigma} \hat{c}^{+}_{i\sigma}\, \hat{c}_{j\sigma} + U \sum_{i} \hat{c}^{+}_{i\uparrow}\, \hat{c}_{i\uparrow}\, \hat{c}^{+}_{i\downarrow}\, \hat{c}_{i\downarrow} \tag{1.11}$$

where $\hat{c}^{+}_{i\alpha}$, $\hat{c}_{i\alpha}$ are, respectively, the creation and annihilation operators for an electron of spin α in the Wannier state at the i^{th} lattice site and the sum $\sum_{<i,j>}$ is restricted to nearest neighbour sites.

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In practice eq.(1.1) can be applied only for the ground state of an interaction-free Hamiltonian. Let us write, after a straightforward manipulation of eq.(1.11) and, as discussed in app.1, choosing a negative definite interaction term :

$$\hat{H} = \hat{T} + V + \frac{U}{2}N \tag{1.12}$$

where

$$\hat{T} = T \sum_{<i,j>,\sigma} \hat{c}^{+}_{i\sigma}\, \hat{c}_{j\sigma}$$

and

$$V = -\frac{1}{2} U \sum_{i} \hat{m}_i\, \hat{m}_i$$

where $\hat{m}_i$ is the magnetization density operator at the site i

$$\hat{m}_i = \hat{c}^+_{i\uparrow}\hat{c}_{i\uparrow} - \hat{c}^+_{i\downarrow}\hat{c}_{i\downarrow} \tag{1.13}$$

Therefore we can separate the potential energy from the kinetic one in the evolution (Fest et al. 1982).

$$e^{-\hat{H}\Delta T} = e^{-\Delta T\frac{U}{2}N}\, e^{-\frac{\Delta T}{2}\hat{T}}\, e^{-V\Delta T}\, e^{-\frac{\Delta T}{2}\hat{T}} + o(\Delta T^3) \tag{1.14}$$

When expression (1.14) is substituted in (1.10), an error in the evaluation of the ground state of $\hat{H}$ will appear in (1.1), due to discretization in time. However formula (1.1) will produce the exact ground state $|\psi'_G>$ of the Hamiltonian

$$\hat{H}' = -\frac{1}{\Delta T}\ln\left(e^{-\frac{\Delta T}{2}\hat{T}}\, e^{-\Delta T\hat{V}}\, e^{-\frac{\Delta T}{2}\hat{T}}\right) + \frac{UN}{2} \tag{1.15}$$

which differ by $o(\Delta T^2)$ from the ground state of $\hat{H}$. In the following I consider ΔT fixed and then I refer to the properties of the Hamiltonian $\hat{H}'$, whose ground state can be written analogously to (1.1)

$$|\psi'_G> = \lim_{N_T\to\infty}\frac{e^{-\hat{H}'N_T\Delta T}|\psi_0>}{||\, e^{-\hat{H}'N_T\Delta T}|\psi_0>\,||} \tag{1.16}$$

Now using the basic relation (1.5) the evaluation of the infinitesimal propagation is:

$$e^{-\hat{H}'\Delta T} = e^{-\frac{U}{2}N\Delta T}\int[d\sigma]\, e^{-\frac{1}{2}\sum_{j=1}^{N_a}\sigma^2_{r_j}}\, e^{-\frac{\Delta T}{2}\hat{T}}\, e^{-(U\Delta T)^{\frac{1}{2}}\sum_r\sigma_r\hat{m}_r}\, e^{-\frac{\Delta T}{2}\hat{T}} \tag{1.17}$$

where

$$[d\sigma] = \prod_{j=1}^{N_a}\frac{d\sigma_{r_j}}{\sqrt{2\pi}}$$

Therefore a many body operator $e^{-\hat{H}'\Delta T}$ is transformed in an integral of product of single particle operators with a considerable advantage from the practical and numerical point of view.

However when substituting the (1.17) in the expression (1.10) a little complication appears because now an index i has to be used for the $\sigma-$variables, in order to distinguish the N_T different Hubbard-Stratonovich transformations (1.17). Using eq.(1.9):

$$e^{-\hat{H}'t} = \int [d\sigma]\, e^{-\frac{1}{2}\underline{\sigma}^2}\; e^{-\frac{UtN}{2}}\,\hat{U}_\sigma \tag{1.18}$$

where

$$\hat{U}_\sigma = \prod_{i=1}^{N_T} e^{-\hat{T}\frac{\Delta T}{2}}\; e^{-(U\Delta T)^{\frac{1}{2}}\sum_r \sigma_r(i)\,\hat{m}_r}\; e^{-\hat{T}\frac{\Delta T}{2}} \tag{1.19}$$

and now $[d\sigma]$ reads:

$$\prod_{i=1}^{N_T}\prod_r \frac{d\sigma_r(i)}{\sqrt{2\pi}} \tag{1.20}$$

whereas formally:

$$\underline{\sigma}^2 = \sum_{i=1}^{N_T}\sum_r \sigma_r^2(i) \tag{1.21}$$

Although the last expression can appear quite cumbersome it is basically, for finite N_T, a multidimensional integral over the $N_T * N_a$ variables σ. Therefore there are many different equivalent ways to get the same transformation, which correspond, for example, to all the possible change of variables in such multidimensional integral.

Usually in the field theory formulation the HST is presented in the continuous limit $\Delta T \to 0$ which surely looks more elegant. Now I prefer to remain with the time discretized version of the HST because it is exactly in this form that it has to be used in computer physics and the continuous limit is an unnecessary formal step. Sometime it can be even confusing to start with the continuous formulation and try to get the discretized version with ambiguous approximation of the continuous limit.

The first observation is that in order to evaluate the integrands in (1.24) there is a big advantage in choosing $|\psi_0>$ as a product of single particle wave functions (for bosons) or as a Slater determinant (for fermions). In these cases $|\psi_0>$ can be very easily propagated through a one-body time dependent operator $\hat{U}_\sigma$ and the calculation of $|\hat{U}_\sigma|\psi_0>$ can be easily done numerically. On the other hand, although expression (1.1) makes possible to have the ground state $|\psi_G>$ starting from an arbitrary trial function, this is an impossible task for size greater than $N_a \simeq 10$ because a function of N particles in a size of N_a sites require the storage of roughly $(N_a)^N$ floating point numbers which are the values of the function $\psi_G(r_1,\ldots,r_N)$ in any possible configuration of r_i. However many informations about the ground state $|\psi_G>$ can be achieved without exceeding the memory possibility of available computers.

As an example consider the ground state energy E_G

$$E_G = < \psi_G \mid H \mid \psi_G > = \lim_{t \to \infty} -\frac{d}{dt} \ln < \psi_0 \mid e^{-Ht} \mid \psi_0 > \tag{1.22}$$

therefore using eq.(1.10) and $t = N_T \Delta T$

$$E_G = \lim_{N_T \to \infty} -\frac{1}{N_T} \frac{d}{d\Delta T} \ln < \psi_0 \mid e^{-H' N_T \Delta T} \mid \psi_0 > \tag{1.23}$$

From the last expression:

$$E_G = \lim_{N_T \to \infty} \frac{1}{N_T} \frac{\int [d\sigma]\, e^{-\frac{1}{2}\underline{\sigma}^2} \; -\frac{d}{d\Delta T} < \psi_0 \mid \hat{U}_\sigma \mid \psi_0 >}{\int [d\sigma]\, e^{-\frac{1}{2}\underline{\sigma}^2} \; < \psi_0 \mid \hat{U}_\sigma \mid \psi_0 >} + \frac{UN}{2} \tag{1.24}$$

An estimation of E_G in expression (1.24) requires the numerical calculation of two multi-dimensional integrals over $A = N_T \times N$ (the degrees of freedom of $\sigma_\tau(i)$) variables with large enough N_T. The straightforward evaluation of an integral like these by one of the standard quadrature formulas is completely out of question except for the very smallest values of A. To see why, suppose that the quadrature allows each coordinate to take on 10 different values (not a very fine discretization), so that the integrand must be evaluated at 10^A points. For a modest value of $A = 60$ and a very fast computer capable of some 10^7 evaluation per seconds, this would take more then 10^{24} times the age of the universe (!). For this reason the choice of a statistical method in order to evaluate the previous integrals is mandatory .

CHAPTER II

Stochastic approach and Langevin dynamics

2.1 Importance sampling

The problem of evaluating a multidimensional integral with a stochastic approach is strictly connected to the idea of importance sampling.

A general integral

$$I = \int [d\sigma]\, P(\sigma) \tag{2.1}$$

can be decomposed in a product of a weight function $w(\sigma)$ time another function $A(\sigma)$:

$$P(\sigma) = A(\sigma)\, w(\sigma) \qquad with \int [d\sigma]\, w(\sigma) = 1 \tag{2.2}$$

Thus the problem is the evaluation of a classical thermal average :

$$I = \frac{\int [d\sigma]\, e^{-\beta V}\, A(\sigma)}{\int [d\sigma]\, e^{-\beta V}} \qquad (with\, \beta = 1) \tag{2.3}$$

where the potential V is defined up to a constant: $V = -\ln w(\sigma) + const.$ With a statistical method we can generate configuration of σ according to the probability function $w(\sigma)$. At this purpose one can use a Monte-Carlo algorithm or a molecular-dynamics strategy: one simply consider the system with σ-degrees of freedom in the fictitious classical potential V.

The decomposition $P(\sigma) = A(\sigma)w(\sigma)$ is arbitrary and $w(\sigma)$ could be chosen as a uniform distribution. However in order to improve the efficiency of the numerical calculation, it is important that w is large when the value of P is large. In this way the configurations "randomly generated" of σ are concentrated about the most important values where w, and hopefully P, is large. This strategy is usually known under the name of "importance sampling".

As it is well known the statistical error of I will be proportional to the inverse square root of the number of sampled configurations p roughly like:

$$\Delta I \propto \frac{(< A^2 > - < A >^2)^{\frac{1}{2}}}{\sqrt{p}} \tag{2.4}$$

The symbol $< A >$ stands for the classical thermal average of an arbitrary function A. Mathematically the "importance sampling" means that we have to choose w and A in such a way that the variance of A is as small as possible.

The most natural choice of V for the evaluation of E_G with the formula (1.24) is:

$$V(\sigma) = \frac{1}{2}\underline{\sigma}^2 - \ln < \psi_0 \mid \hat{U}_\sigma \mid \psi_0 > \tag{2.5}$$

with $A_E(\sigma) = -\frac{1}{N_T}\frac{d}{d\Delta T}\ln < \psi_0 \mid \hat{U}_\sigma \mid \psi_0 >$. In this way one can write:

$$E_G = \frac{UN}{2} + < A_E > \tag{2.6}$$

The potential V in the preceding expression (eq. 2.5) is classical and couples the classical degrees of freedom σ. It has not to be confused with the real potential acting on the true quantum many-body system.

However the last choice of V (eq. 2.5) is affected by a considerable drawback. In fact $< \psi_0|\hat{U}_\sigma|\psi_0 >$ is not always a positive real number because $\hat{U}_\sigma$ in (1.19) which is the product of Hermitian positive definite matrices is in general neither Hermitian nor positive definite. For field configurations which vary slowly enough in time so that the adiabatic approximation can be used in computing the product of positive definite matrices in (1.19) $\hat{U}_\sigma$ is still positive definite. However the field configurations that dominates the functional integral are not in general slowly varying. Therefore even if we limit ourselves to a real wave function $|\psi_0>$ ($\hat{U}_\sigma$ is still a real operator) $< \psi_0|\hat{U}_\sigma|\psi_0 >$ can change its sign. Consequently the potential $V(\sigma)$ is not a real potential. On the other and one can consider in expression (2.5) the logarithm of the absolute value of $< \psi_0|\hat{U}_\sigma|\psi_0 >$:

$$V(\sigma) = \frac{1}{2}\underline{\sigma}^2 - \ln \mid < \psi_0 \mid \hat{U}_\sigma \mid \psi_0 > \mid \tag{2.7}$$

However in the surface where $< \psi_0|\hat{U}_\sigma|\psi_0 >= 0$ the potential V is infinite. For any dynamical evolution both statistical or deterministic with potential V the mentioned surface cannot be crossed. In principle, using the L.E. in the continuous limit, the average of A_E is restricted in a region with defined sign of $< \psi_0|\hat{U}_\sigma|\psi_0 >$. A way to overcome the latter difficulties is obtained using a new definition of the potential which is always real and has no infinite potential barriers :

$$V' = \frac{1}{2}\underline{\sigma}^2 - \ln \| U_\sigma \mid \psi_0 > \| \tag{2.8}$$

From which:

$$E_G = \frac{UN}{2} + \frac{< S(\sigma) - \frac{\partial}{\partial \Delta T} \ln < \psi_0 \,|\, \hat{U}_\sigma \,|\, \psi_0 > >_{V'}}{< S(\sigma) >_{V'}} \tag{2.9}$$

where

$$S(\sigma) = \frac{< \psi_0 \,|\, \hat{U}_\sigma \,|\, \psi_0 >}{|| \hat{U}_\sigma \,|\, \psi_0 > ||} \quad (|S(\sigma)| \leq 1) \tag{2.10}$$

Unfortunately the potential V' does not make a good "importance sampling" in the sense discussed before. In fact it does not depend on the angle that the propagated wave function $\hat{U}_\sigma|\psi_0>$ forms with the trial function $|\psi_0>$. Therefore $S(\sigma)$ freely fluctuates with a variance of the order of 1. However the statistical average of many interesting quantities (like the energy E_G) over the potential V can converge to the exact value for $NT \longrightarrow \infty$ even with the restriction of sampling only the positive values of $< \psi_0|\hat{U}_\sigma|\psi_0 >$.

Numerical tests confirm that the statistical error produced by the potential V' was one or two order of magnitude larger then the one obtained with the previous potential V.

2.2 Langevin dynamics

According to the definition of the potential V in (2.5) the variables σ are coupled by means of a long range interaction. In fact it is enough to change only one σ_r and the forces acting on any degrees of freedom will also change due to the variation of $< \psi_0|\hat{U}_\sigma|\psi_0 >$ (see 1.19). In this case a Monte-Carlo scheme generating population of σ according to the distribution e^{-V} is not as efficient as in the case V is short-ranged. In fact a random change of σ, using the Metropolis algorithm, will require the evaluation of the new $< \psi_0|\hat{U}_\sigma|\psi_0 >$ by means of NN_T multiplications of matrices $N_a \times N_a$. This requires a quite large computer time for only one new configuration (which can be even rejected).

Actually it is possible to reduce the very large factor (Blankenbecker et al. 1981) N_T but for numerical reasons this tricks cannot be often applied, that is $\hat{U}_\sigma$ must be computed from scratch any $\simeq 10N$ new configurations.

If the time required for any new evaluation of V is very large the numerical advantage of the Monte-Carlo algorithms is lost, compared with the methods which use a molecular dynamics strategy for multi-dimensional integral as in (1.9). As an example let us consider in detail the Langevin dynamic scheme (Parisi and Yougshi 1981, Gunsteren and Berendsen 1982) described by the following differential equations:

$$\frac{d\,\sigma_{r_j}(i)}{ds} = F_s(r_j, i) + \eta_{j,i}(s) \tag{2.11}$$

where

$$F_s(r_j,i) = -\frac{\partial V}{\partial \sigma_{r_j}(i)} \tag{2.12}$$

and $\eta_{j,i}(s)$ are random gaussian distributed variables with 0 mean and variance:

$$< \eta_{j,i}(s)\,\eta_{j',i'}(s') >= 2\beta^{-1}\,\delta_{jj'}\,\delta_{ii'}\,\delta(s-s') \tag{2.13}$$

($\beta = 1$ in our choice of V eq.2.7). If we impose a boundary condition at $t = 0$ the solution of eq.(2.11) is uniquely given in terms of η, let us call it $\sigma^{\eta}_{r_j}(i,s)$. It is a well known from statistical mechanics that for large s one has

$$< \sigma^{\eta}_{r_j}(i,s)\,\sigma^{\eta}_{r_{j'}}(i',s) > \longrightarrow < \sigma_{r_j}(i)\,\sigma_{r_{j'}}(i') >_V \tag{2.14}$$

i.e. the equal time non-equilibrium correlations (the brackets in the left hand side of eq. (2.14) indicate the mean value over η) tend to the equilibrium one for large time s. It has been shown (Parisi and Yougshi 1981) that the convergence in the last expression is exponential. Hence after a long time such that the stochastic evolution lose memory of the initial condition the dynamic will generate sample of $A(\sigma)$ according to the desired probability distribution e^{-V}.

In practice the average of any stochastic variable $< A >$ can be computed by numerically solving the Langevin Equation (L.E.), and using the following assumption:

$$< A >= \lim_{s\to\infty} \frac{1}{s}\int_0^s A(s')\,ds' \tag{2.15}$$

which is a generalization of the previous equation (2.14). This assumption follows from eq.(2.14) if the solutions of eq.(2.11) are "ergodic", that is they cover all the phase space of the σ degrees of freedom. This is not the case in general because, as discussed before, the phase space can contain disconnected domains separated by infinite potential barriers (as for the potential V in eq.2.7). Indeed a Monte-Carlo algorithm or a discretized version of such dynamical evolution can even cross an infinite potential barrier because, with an iterative statistical algorithm, some random step can provide a jump from one side to another side of the potential barrier.

The basic step to solve the L.E. is the $s-$time discretization which involves an error depending on the time step Δs and on the algorithm used to discretize the L.E. (first order, second order, ..., n^{th} order in Δs). Integrating eq.(2.11) we obtain

$$\sigma_{r_j}(i,s+\Delta s) - \sigma_{r_j}(s) = \int_s^{\Delta s+s} F_s(r_j,i)\,ds' + \int_s^{s+\Delta s} \eta_{j,i}(s')\,ds'. \tag{2.16}$$

It is convenient to introduce discrete stochastic variables $z^k_{j,i}$

$$\int_{k\Delta s}^{(k+1)\Delta s} \eta_{j,i}(s')\,ds' \;=\; z^k_{j,i}\,\sqrt{2\Delta s\,\beta^{-1}} \quad s \;=\; k\Delta s. \tag{2.17}$$

According to eqs. (2.13) and (2.16) $z^k_{j,i}$ are uncorrelated normal-distributed numbers with mean $< z^k_{i,j} >= 0$ and variance $< z^{k\,2}_{i,j} >= 1$

The first order algorithm to solve the L.E. is obtained approximating

$$\int_{s}^{s+\Delta s} F_{s'}(r_j,i)\,ds' \;=\; F_s(r_j,i)\,\Delta s + \,o(\Delta s^2) \tag{2.18}$$

and neglecting terms of order Δs^2:

$$\sigma_{r_j}(i,s+\Delta s) \;=\; \Delta s\; F_s(r_j,i) \;+\; z^k_{i,j}\,\sqrt{2\,\beta^{-1}\,\Delta s} \;+\; \sigma_{r_j}(i,s). \tag{2.19}$$

More accurate algorithms are easily obtained improving the approximation on (2.18):

$$\int_{s}^{s+\Delta s} F_{s'}(r_j,i)\,ds' \;=\; \int_{s}^{s+\Delta s} \Big(F_s(r'_j,i) \;+\; (s'-s)\,\dot{F}_s(r_j,i)\Big)\,ds' \;+\; o(\Delta s^3) \tag{2.20}$$

Using a finite difference expression for F_s:

$$\frac{F_s(r_j,i) \;-\; F_{s-\Delta s}(r_j,i)}{\Delta s} \tag{2.21}$$

and straightforward manipulation, the 2^{nd} order algorithm reads :

$$\sigma_{r_j}(i,s+\Delta s) \;=\; \sigma_{r_j}(i,s) \;+\; \Delta s\,(\frac{3}{2}F_s(r_j,i) \;-\; \frac{1}{2}\,F_{s-\Delta s}(r_j,i)) \;+\; z_{i,j}\,\sqrt{2\beta^{-1}\,\Delta s}. \tag{2.22}$$

The algorithm requires the knowledge of the forces at the preceding step.

We indicate with s_0 the time necessary to reach the equilibrium distribution. the s-time averages (2.15) are the calculated according to the following equation:

$$< A >= \frac{1}{M} \sum_{s=s_0}^{s_0+(M-1)\Delta s} A(s) \tag{2.23}$$

In order to have an estimation of the statistical error we also calculate the variance of A:

$$\frac{1}{M} \sum_{s=s_0}^{s_0+(M-1)\Delta s} [A^2(s) - \,< A >^2]^{\frac{1}{2}} \;=\; \Delta A \tag{2.24}$$

The statistical error of the variable A will behave roughly as :

$$A = \frac{\Delta A}{\sqrt{\frac{s - s_0}{\tau}}} \tag{2.25}$$

where τ is the typical correlation time in the Langevin dynamical evolution (in this case $\tau \simeq 1$). From eq.(2.25) it is clear why a more accurate discretization of the L.E. is useful. In fact it allows to work with a larger time step Δs so that the equilibrium can be more rapidly reached and from (2.25) one has a better statistical error with the same number of iterations.

In the previous iteration schemes eqs. (2.19) and (2.22) there is a basic ingredient: the generation of random gaussian numbers $z^k_{i,j}$. Indeed it is not obvious how to generate "random" numbers on deterministic computers, so that these numbers are usually called pseudo-random numbers.

An efficient way for generating normally distributed numbers is described in app.2.

CHAPTER III

Positiveness of the statistical weight

In the previous chapter applied the Langevin dynamics (see eqs.2.18-2.21) to a classical statistical system which interacts via a potential (2.7): the numerical simulation of this classical system allows to investigate the quantum-mechanical properties of a system of interacting particles. However it should be kept in mind that the potential defined in eq.(2.7) is a fictitious potential, which has very few in common with the quantum-mechanical potential acting on the real quantum particles.

The degrees of freedom of the classical system are $2N_T N_a$, where N_a is the number of spatial lattice sites and N_T, the number of imaginary time steps must be chosen large enough to guaranty the convergence. Hence the Hubbard Stratonovich transformation allows to map (see eq.1.18) a quantum system of a finite number of degrees of freedom (H has a finite dimension) at $0°K$ on a classical system, at finite temperature with large enough number of degrees of freedom such that the convergence is guaranteed in eq.(1.22).

It is natural at this point to characterize the thermodynamic properties of this classical system by its classical partition function

$$Z = \int [d\sigma]\; e^{\frac{1}{2}\sigma^2} \; < \psi_0 \,|\, \hat{U}_\sigma \,|\, \psi_0 > = < \psi_0 \,|\, e^{-H' N_T \Delta T} \,|\, \psi_0 > \; > \; 0 \qquad (3.1)$$

where the equality sign holds using eqs.(1.19-1.21) and the inequality one because $e^{-\hat{H}' N_T \Delta t}$ is a positive definite operator. Analogously the corresponding free energy is:

$$F = \lim_{NT \to \infty} \frac{1}{NT} \ln Z \qquad (3.2)$$

From the knowledge of this free energy F one can evaluate many quantities important for the quantum mechanical system. As an example the ground state energy, using eq.(1.24) and the definition of Z in eq.(3.1), can be written as a simple derivative of the free energy (3.2) (see 1.22): $E_G = -\frac{d}{d\Delta T} F$.

However Z is not a true partition function of any classical system because the integrand in (3.1) is not always positive definite for any field configuration and cannot represent a probability distribution. It is convenient to define:

$$Z = Z_+ - Z_- \qquad (3.3)$$

where

$$Z_+ = \int [d\sigma]\, e^{-V(\sigma)} \Theta \left(< \psi_0 \,|\, \hat{U}_\sigma \,|\, \psi_0 > \right) \tag{3.4}$$

and

$$Z_- = \int [d\sigma]\, e^{-V(\sigma)} \Theta \left(- < \psi_0 \,|\, \hat{U}_\sigma \,|\, \psi_0 > \right) \tag{3.5}$$

with

$$V = \frac{1}{2}\sigma^2 - \ln | < \psi_0 \,|\, \hat{U}_\sigma \,|\, \psi_0 > | \tag{3.6}$$

and Θ is the step function. In principle, with the potential (3.6) any classical average $< A >$ corresponding to a suitable derivative of the free energy F (eq.3.2) can be expressed in the following way:

$$< A > = \frac{< A >_+ - \dfrac{Z_-}{Z_+} < A >_-}{1 - \dfrac{Z_-}{Z_+}} \tag{3.7}$$

where the $+$ and $-$ sign indicate the average of the function a in a region of defined sign.

In expression (3.7) the ratio between the two partition function can be obtained by evaluating the average-determinant sign r (with the potential 3.6):

$$r = < sign \left(< \psi_0 \,|\, \hat{U}_\sigma \,|\, \psi_0 > \right) > \tag{3.8}$$

from which the ratio between the two partition function is easily obtained:

$$\frac{Z_-}{Z_+} = \frac{1 - r}{1 + r} \tag{3.9}$$

Although a Langevin dynamic is very efficient for the computation of averages in a region of defined sign ($< A >_-$ and $< A >_+$ in 3.7) the calculation of the $< \psi_0 \,|\, \hat{U}_\sigma \,|\, \psi_0 >$ average sign (3.8) gives some trouble. In fact, as we have already mentioned, the dynamical evolution always remains in a positive or a negative region for a continuous Langevin evolution. For a discrete one (eq. 2.19-2.22) the probability of a jump is smaller and smaller as far as the time step tends to zero. This means that a very large computer time is needed to estimate the average-determinant sign with a small enough statistical error. It would be very convenient (as some authors guessed Blankenbecker et al. 1981) if for large N_T only the positive sign is statistically dominant ($r \to 1$). Actually in the following

we can give a less restrictive condition to average only in a region of a definite sign. The last property is not verified only when the average $< \psi_0 \,|\, \hat{U}_\sigma \,|\, \psi_0 >$ sign vanishes in the infinite N_T limit. Now r is –from relation (1,9) and inequality $Z = Z_+ - Z_- > 0$ (see eq.3.1-3.2)– a number between 0 and 1.

$$0 < r \leq 1 \tag{3.10}$$

Moreover from eq.(1.9) it simply follows that Z can be written as:

$$Z = Z_+ \left(1 - \frac{Z_-}{Z_+}\right) = Z_+ \frac{2r}{1+r} \tag{3.11}$$

Using the definition of F and the preceding relation (3.11)

$$\begin{aligned} F(N_T) &= \frac{1}{N_T} \ln Z(N_T) = \frac{1}{N_T} \ln Z_+(N_T) + \frac{1}{N_T} \ln(\frac{2r}{1+r}) \\ &= F^+(k) + \frac{1}{N_T} \ln(\frac{2r}{1+r}) \end{aligned} \tag{3.12}$$

By taking the limit in both sides of the preceding equality one easily get that:

$$\lim_{NT \to \infty} F^+ = \lim_{NT \to \infty} F \;\; if \lim_{NT \to \infty} r \neq 0 \tag{3.13}$$

The latter relation means that whenever $\lim_{NT \to \infty} r \neq 0$ it is possible to restrict the statistical averages over a region of positive $< \psi_0 \,|\, \hat{U}_\sigma \,|\, \psi_0 >$ for quantities that can be expressed as suitable derivatives of the free energy (3.2).

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Analogously it is simple to show that F_+ tends to F_- for large N_T unless the average determinant sign converges exactly to 1.

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It is very simple to realize why for very small U (indeed $(U\,\Delta T)^{\frac{1}{2}} \ll E_{gap}(U=0)\,\Delta T$ the partition function Z is prevalently positive. In fact $\hat{U}_\sigma$ acts, in this case, as an adiabatic operator and, as well known, $< \psi_0 | \hat{U}_\sigma | \psi_0 >> 0$ regardless for less relevant configuration with very large σ. Indeed $Z = Z_+ \,\forall\, NT$ in a neighborhood of U if $|\sigma| < \Lambda$ and $(U\Delta T)^{\frac{1}{2}} \ll E_{gap}\Delta T$. When the HST is performed with the condition $|\sigma| < \Lambda$ the error in evaluating F is negligible if Λ is sufficiently large). Then F and F_+ (the existence of the thermodynamic limit for F_+ has been shown in app.2) surely coincide in a neighbourhood

of $U = 0$. If F_+ is an analytical function of U (F is analytical for a finite system) F and F_+ coincide for any value of the interaction for a well known property of analytical functions. Suppose that F and F_+ are different for some particular value of the interaction, then F_+ is a singular free energy and a phase-transition occurs for the classical system described by the σ degrees of freedom.

From the preceding discussion, after calculating the averages in the regions of defined sign, it is important to check whether r in eq.(3.12) does not converge to 0. In this case we can identify the total average of A with the one restricted in the positive or negative regions. In this way the statistical error is considerably reduced. However, if the number r is very small, the statistical error and the extrapolation $N_T \to \infty$ must be performed within a tolerance less then the value of r itself in order to be sure of its non vanishing limit. Using the results given in app.1b and:

$$r = \frac{S_{N_T}}{2 - S_{N_T}} \tag{3.14}$$

Then either $r \to 0$ and in this case the convergence is exponential or:

$$\lim_{N_T \to \infty} r > \frac{< \psi_0 \mid \psi_G >^2}{2 - < \psi_0 \mid \psi_G >^2} \tag{3.15}$$

The latter property now allows to simplify the problem of the estimation of r in a numerical feasible way. In fact, in the case $r \to 0$, the convergence is exponential and a reasonable accuracy can be achieved without a large value of N_T. On the other hand if the trial wave function $|\psi_0>$ is a good one (when $< \psi_0 | \psi_G >$ is large enough) the possibility to distinguish whether (3.15) holds is easier.

CHAPTER IV

The algorithm

4.1 Numerical stability and Graham-Schmidt orthogonalization

In order to build up an iterative algorithm it is convenient to choose $|\psi_0>$ as a Slater determinant (or analogously the sum of few Slater determinants)

$$|\psi_0> = \frac{1}{\sqrt{N!}} det\,[\varphi_m(r_j)] \tag{4.1}$$

where $\varphi_m, m = 1,\ldots,N$ are N independent orthogonal orbitals and r_j are the coordinates of the N particles.

In fact the evolution of a slater determinant trough the single particle time dependent potential $\hat{U}_\sigma\,|\psi_0>$ is again a single particle determinant state.

Moreover $\hat{U}_\sigma$ is the product of single particle operators, then the evolution of a many body Slater determinant through $\hat{U}_\sigma$ simplifies in solving the evolution of the N single particle orbitals

$$\varphi_m(T) = \hat{U}_\sigma \varphi_m(0)\ for\, i = 1,\ldots,N \tag{4.2}$$

This problem is numerically accessible by an iterative algorithm, using the time discretized expression of $\hat{U}_\sigma$

$$\hat{U}_\sigma = \prod_{i=1}^{N_T} \hat{U}_{\sigma(i)} \tag{4.3}$$

In fact from eq. (1.19)

$$\hat{U}_{\sigma(k)} = e^{-\hat{T}\frac{\Delta T}{2}}\, e^{-\sum_r \sigma_r(k)\,\hat{m}_r\,\sqrt{U\,\Delta T}}\, e^{-\hat{T}\frac{\Delta T}{2}} \tag{4.4}$$

is a product of a single particle operators which are diagonal either in Fourier space ($\hat{T}$) or in real space ($\hat{m}_r$). One can use the Fourier transform algorithm (Fest et al. 1982) to evaluate:

$$\varphi_i^{T+\Delta T} = \hat{U}_{\sigma_r}(k)\,\varphi_i^T \ with\ k = \frac{T}{\Delta T}\ ,\ i = 1,\ldots,N \tag{4.5}$$

In this way $|\psi_i(k\Delta T)>$ for $k = 1,\ldots,N_T$ can be computed by means of $N_T N N_a \ln_2 N_a$ operations. The mentioned algorithm is obtained by going back and forth between Fourier and real space where $\hat{T}$ or $\hat{m}_r$ are diagonal operators.

Troubles arise because $\hat{U}_{\sigma(i)}$ are not unitary (orthogonal) operators. Therefore after repeating many times the step (4.5) an orthogonal basis set $\varphi_i(r)$ $i = 1, \ldots, N$ will no longer remain orthogonal. This circumstance can produce a numerical instability of the algorithm. The simple reason of such instability is because the fermionic ground state can be considered as an excited state (with the right simmetry) of a many-body hamiltonian; its true ground state being a boson-symmetric wavefunction. In fact when the orbitals freely propagate, after long time, they they are led spontaneously to the bosonic ground state.In this way the numerical information of the fermionic state is gradually lost until the Slater determinant exactly vanishes because of round-off error. Therefore, in order to have a stable propagation, we have to rewrite, any few steps, the Slater determinant which is at the time T:

$$|\psi >^T = det\, \varphi_m^T(r_j) \tag{4.6}$$

in terms of an orthogonal basis set. This is always possible with a transformation

$$\varphi_m^T = \sum_n U_{m,n}\, \tilde{\varphi}_n^T \tag{4.7}$$

where the matrix $U_{m,n}$ is chosen in such a way that $< \tilde{\varphi}_m^+ | \tilde{\varphi}_n^+ >= \delta_{m,n}$ provided φ_m^T are linearly independent orbitals. This is always satisfied because $|\psi_0 > \neq 0$ and $|\psi_T >$ results from the propagation of $|\psi_0 >$ by means of positive definite matrices; then $|\psi^T > \neq 0$ and $\{\varphi_m^T\}$ are linearly independent functions (otherwise $|\psi^T >= 0$). The matrix $U_{m,n}$ is not univocally determined by the previous condition. A convenient choice is to use the Graham- Schmitd orthogonalization scheme because, in this case, $U_{m,n}$ is a triangular matrix.

Now from (4.6) and (4.7) $|\psi^T >$ can be written as

$$|\psi >^T = det \left[\sum_n U_{m,n}\, \tilde{\varphi}_n^T(r_j) \right] \tag{4.8}$$

this means that for any values of the coordinates $r_j, |\psi >^T$ is the determinant of the product of two square matrices: $U_{m,n}$ and $\tilde{\varphi}_n^T(r_j)$. Therefore using that the determinant of the product of two matrices is equal to the product of the two determinants, one easily gets that:

$$|\psi >^T = \| \psi \|\, |\psi' >^T \tag{4.9}$$

where $||\psi|| = det\, U_{m,n}$ and $|\psi' >$ is again a Slater determinant made up by orthonormal orbitals:

$$|\psi' >^T = det\, \tilde{\varphi}_k^T(r_j) \tag{4.10}$$

In this way from some time on, the propagation of the many body wave function is:

$$|\psi>^{T+\Delta T} = \hat{U}_{\sigma(k)} \left\| |\psi^T> \right\| |\psi'>^T = \left\| |\psi>^T \right\| U_{\sigma(k)} |\psi'> \tag{4.11}$$

Therefore we again have to propagate a Slater determinant and one can proceed as before until the numerical stability will require another orthogonalization. Such a strategy has been shown numerically to be very useful. One of the reasons is that in this way one easily overcome the problem of the overflow (underflow). In fact the norm of the propagated wave function can become very large (small) when the time T is large. We can store the function $|\psi>^T$ by the values of $\ln ||\psi^T||$ and N independent single particle wave functions.

At any orthogonalization we have only to correct the storage of the norm in the following way:

$$[\ln ||\psi||]^{T^+} = [\ln ||\psi||]^{T^-} + \ln det\, U_{i,j} \tag{4.12}$$

where T^+ and T^- indicates formally after and before the orthogonalization. It is clear that it is very difficult to reach an overflow with an operation like the (4.12) and on the other hand for many quantities (like the energy in eq. (1.24) only the knowledge of $\ln \left\| |\psi> \right\|$ is required.

Another more important reason for orthogonalizing is the following. Suppose to have a Slater determinant $|\psi>$ containing two functions $|0>$ and $|1>$ which propagates under a single particle time independent Hamiltonian $\hat{h}$. Here $\hat{h}$ is Hermitian with lowest eigenvalues E_0, E_1 $(E_0 < E_1)$ and corresponding eigenvectors $|\tilde{0}>$and $|\tilde{1}>$. Suppose now that $|0>$ coincides with $|\tilde{0}>$ and $|1>$ has a very small component of $|\tilde{0}>$: $|1>=|\tilde{1}>+\alpha|\tilde{0}>$. Now in principle

$$\lim_{t\to\infty} \frac{e^{-\hat{h}t}|\psi>}{\left\| e^{-\hat{h}t}|\psi> \right\|} \tag{4.13}$$

has to give the ground state of $\hat{h}$ (see eqs.1.1-1.3). The single particle evolution of $|0>$ and $|1>$ reads:

$$|0>^t = e^{-E_0 t}|\tilde{0}>$$

$$|1>^t = e^{-E_1 t}|\tilde{1}> + \alpha e^{-E_0 t}|\tilde{0}> \tag{4.14}$$

therefore suppose that the computer can store P figures and $|\tilde{0}>$ or $|\tilde{1}>$ are of the same order of magnitude. After a time such that

$$t > \frac{P \ln 10 - \ln \alpha}{E_1 - E_0} \tag{4.15}$$

the information about $|\tilde{1}>$ is completely lost because:

$$|1>^t = e^{-E_0 t}\left[|\tilde{0}> + e^{(E_0-E_1)t-\ln\alpha}|\tilde{0}>\right] \tag{4.16}$$

and for such computer $1+10^{-P}=1$. Hence numerically the ground state of $\hat{h}$ would become the vacuum. In fact the Slater determinant at a time

$$t = \frac{P\ln 10 - \ln\alpha}{E_1 - E_0} \tag{4.17}$$

contains two linear dependent functions.

From eq.(4.17) the mentioned instability depend on the gap between the two energy in the single particle hamiltonian. Of course when dealing with many electrons, the statistical gap of the instantaneous operator $\hat{U}_\sigma$ can be very large ($\simeq N_a\sqrt{U\Delta T}$) because it is the difference between the instantaneous ground state energy of $\hat{U}_\sigma$ and the N^{th} excited one. So far it is convenient to orthogonalize quite frequently in order to preserve some significant digits in the calculation.

The mentioned numerical instability has something to do with a physical phenomena. In fact when the single particle wave functions are free to propagate they are spontaneously led to the boson ground state just because of the roundoff error. I believe that the orthogonalization is a necessary step if one wants to preserve the antisymmetry of the fermionic ground state.

As far as the computation speed is concerned I have to remind that the time required for a Graham–Smith orthogonalization costs an amount of N^2N_a floating point multiplications. It is therefore much more expansive than the propagation algorithm (4.5) but one has to consider that it is not necessary at all to perform an orthogonalization at any step. We can see in the following sections that once an orthogonalization is performed, it is possible to have a sample of many statistical quantities with the same amount of computer time.

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4.2 FORCES

The forces in expressions (2.19,2.22) of the statistical system composed by the N_a-dimensional interacting oscillators $\sigma_{r_j}(i)$ are given:

$$F_{r_j}(i) = -\frac{\partial}{\partial\sigma_{r_j}(t)} V(\sigma) = -\sigma_{r_j} + \frac{\partial}{\partial\sigma_{r_j}} \ln < \psi_0 \mid \hat{U}_\sigma \mid \psi_0 > \tag{4.18}$$

We consider the trial wave function ψ_0 made up by $N^\uparrow$ spin up orbitals and $N^\downarrow$ spin down ones. As mentioned before, $\hat{U}_\sigma$ acts independently over the sets of functions with defined spin projections

$$|\varphi^\uparrow_m > \quad |\varphi^\downarrow_n >$$

Therefore it is simple to show that

$$< \psi_0 | \hat{U}_\sigma | \psi_0 > = det < \varphi^\uparrow_m | \hat{U}_\sigma | \varphi^\uparrow_n > det < \varphi^\downarrow_m | \hat{U}_\sigma | \varphi^\downarrow_n > \tag{4.19}$$

and the problem of computing the forces is completely decoupled in spin space. As a consequence:

$$F_{r_j}(i) = -\sigma_{r_j} + \frac{\partial}{\partial\sigma_{r_j}(i)} \ln det < \varphi^\uparrow_m \mid \hat{U}_\sigma \mid \varphi^\uparrow_n > + \frac{\partial}{\partial\sigma_{r_j}(i)} \ln det < \varphi^\downarrow_m \mid \hat{U}_\sigma \mid \varphi^\downarrow_n > \tag{4.20}$$

The derivative in the last expression affects only the propagator U_σ at the time slice i. Such derivative, if done in a non convenient way, requires the computation of at least one determinant for each degrees of freedom $N_T N_a$. From now on we consider in detail the calculation of the spin up term in eq.4,20 because the remaining term, concerning the spin down orbitals, can be analogously treated. For a non convenient calculation, say with a numerical estimation of the derivatives in eq.(4.20), the calculation takes the order of $N_T N_a M^3$ operations. In order to reduce such waste of time we note that setting:

$$A_{m,n}(\sigma) = < \varphi^\uparrow_m \mid \hat{U}_\sigma \mid \varphi^\uparrow_n > \tag{4.21}$$

The determinant of any matrix can be written formally

$$det\, A = e^{tr \ln A}$$

Therefore the second term in the R.H.S. of eq.(4.20) now becomes:

$$-\frac{tr\, \ln A^-}{\partial\sigma_r(i)} = -tr\, \frac{\partial A}{\partial\sigma_r(i)} A^{-1} = \sum_{m,n} \left[\frac{\partial A}{\partial\sigma_r(i)}\right]_{mn} A^{-1}_{nm} \tag{4.22}$$

The explicit expression of $\frac{\partial}{\partial\sigma_r(i)} A$ can be worked out introducing the back and forth propagated orbitals which are calculated at the time $\left(i - \frac{1}{2}\right)\Delta T$, $i = 1, \ldots, N_T$ because the derivative with respect to a variables $\sigma(\vec{r}_j, i)$ affects the propagator at the mentioned time step. These back and forth propagated orbitals can be calculated with an iterative scheme :

$$\varphi_{>,m}(i) = e^{-\sum_r \sqrt{U\Delta T}\,\sigma_r(i)\,\hat{c}_r^+\,\hat{c}_r}\, e^{-\Delta T\,\hat{T}}\, \varphi_{>,m}(i-1)$$

$$\varphi_{>,m}(1) = e^{-\sum_r \sqrt{U\Delta T}\,\sigma_r(1)\,\hat{c}_r^+\,\hat{c}_r}\, e^{-\frac{\Delta T}{2}\hat{T}}\, \varphi_{>,m}(0) \tag{4.23}$$

$$\varphi_{<,m}(i-1) = e^{-\Delta T\,\hat{T}}\, e^{-\sum_r \sqrt{U\Delta T}\,\sigma_r(i)\,\hat{c}_r^+\,\hat{c}_r}\, \varphi_{<,m}(i)$$

$$\varphi_{<,m}(N_T) = e^{-\frac{\Delta T}{2}\hat{T}}\, \varphi_m(0) \tag{4.24}$$

where $\varphi_m(0)$ are the one particle orbitals corresponding to the given many body wave function $|\psi_0>$.

Now using (4.21) and the previous definition (4.23) and (4.24):

$$\left[\frac{\partial}{\partial\sigma_r(i)} A\right]_{m,n} = -\sqrt{U\,\Delta T}\, <\varphi^{\uparrow}_{<,m}(i)\,\hat{c}_r^+\,\hat{c}_r\,\varphi^{\uparrow}_{>,n}(i)> \tag{4.25}$$

The previous expression for each m, n becomes very simple in real space where it is the product of two real functions at the site point $\underline{r}$. In order to calculate the forces acting on all σ we need an inverse operation (M^3 operations) the calculation of the forth and back propagated orbitals at each time $i = 1, \ldots, N_T$ ($N_T\,N\,N_a\,\ln(N_a)$ operations) and via formula (4.22) the final expression with $N^2 N_T N_a$ operations.

Apparently we have got only a little advantage (a factor N) with respect to the previous direct method. Actually a further improvement can be obtained by moving the sum operation into the vector brackets in (4.22). Hence using (4.25):

$$tr\,\frac{\partial}{\partial\sigma_r(i)} A^{-1} = \sum_m -\sqrt{U\,\Delta T}\, <\sum_n A^{-1}_{m,n}\,\varphi_{<,n}(i)|\,\hat{c}_r^+\,\hat{c}_r\,|\varphi_{>,m}(i)> \tag{4.26}$$

Once we compute the set of states (a change of basis needs $N^2 N_a$ operations) for $i = N_T$

$$\varphi^{A^{-1}}_{<,m}(i) = \sum_n A^{-1}_{m,n}\,\varphi_<(i)$$

The propagation of $\varphi_{<}^{A^{-1}}$ can be performed in the same footing as in (4.23) because the single particle operators in (4.23) are linear, then:

$$\varphi_{<,m}^{-1}(i-1) = e^{-\Delta T \hat{T}}\, e^{-\left[\sqrt{U\Delta T}\sum \sigma_r(i)\,\hat{c}_r^{+}\,\hat{c}_r\right]}\,\varphi_{<,m}^{A^{-1}}(i) \tag{4.27}$$

Hence we are finally left with only $NN_a \ln(N_a) N_T + N^2 N_a + N^3$ operations for computing all the forces and we saved a factor NN_T with respect to the first algorithm.

The last algorithm is very fast but the numerical stability, discussed in the previous chapter, is not taken into account. At this purpose we need to orthogonalize any say I_L steps ($N_T = I_L \times I_P$ where I_P is the number of orthogonalizations used for the back and forth propagation of the orbitals). In this way we lose the possibility to write the matrix $A_{m,n}$ in terms of the trial orbitals. However we note that the previous arguments can be applied between two contiguous orthogonalizations because in any interval like that the single particle wave functions propagate independently. In fact from the time $(n_T - 1)I_L\,\Delta T$ to the time $n_T I_L \Delta T$ one can write in (4.18)

$$< \psi_0 \,|\, \hat{U}_\sigma \,|\, \psi_0 > = < \tilde{\psi}_<(n_T) \,|\, \prod_{i=(n_T-1)I_L+1}^{n_T\, I_L} \hat{U}_{\sigma(i)} \,|\, \tilde{\psi}_>(n_T - 1) > \; N_{n_T}^{<}\, N_{n_T-1}^{>} \tag{4.28}$$

where $|\tilde{\psi}_>(n_T)>$ and $|\tilde{\psi}_<(n_T)>$ are proportional to the back and forth propagated many body states $|\psi_>(n_T)>$, $|\psi_<(n_T)>$ expressed after orthogonalization by N orthogonal orbitals $\tilde{\varphi}_{<,mj}$ $\tilde{\varphi}_{>,m}$ and norms $N_{n_T-1}^{>}$ and $N_{n_T}^{<}$ (see sect.1)

$$\begin{aligned} |\,\psi_>(n_T)> &= \prod_{i=1}^{n_T\, I_L} \hat{U}_{\sigma(i)} \,|\, \psi_0 > = N_{n_T}^{>} \,|\, \tilde{\psi}_>(n_T) > \\ |\,\psi_>(n_T)> &= \prod_{i=N_T}^{n_T\, I_L - 1} \hat{U}_{\sigma(i)} \,|\, \psi_0 > = N_{n_T}^{<} \,|\, \tilde{\psi}_<(n_T) > \end{aligned} \tag{4.29}$$

It is clear now that in the previous expressions (4.22) and (4.25) the matrix A must be substituted with:

$$A_{m,n} = < \tilde{\varphi}_{<,m}(n_T) \,|\, \prod_{i=(n_T-1)I_L+1}^{n_T\, IL} \hat{U}_{\sigma(i)} \,|\, \tilde{\varphi}_{>,n}(n_T - 1) > \tag{4.30}$$

and (4.23) and (4.24) slightly modify by changing $\varphi_m(0)$ with $\tilde{\varphi}_{<,m}(n_T)$ and $\tilde{\varphi}_{>,j}(n_T - 1)$ respectively for the initialization of the iteration scheme:

$$\varphi_{<,m}(n_T I_L) = e^{-\frac{\Delta T}{2}\hat{T}}\,\tilde{\varphi}_{<,m}(n_T) \tag{4.31}$$

$$\varphi_{>,m}((n_T-1)I_L+1) = e^{-\sqrt{U\Delta T}\sum_r \sigma_r((n_T-1)I_L+1)\,\hat{c}_r^+\,\hat{c}_r}\; e^{-\frac{\Delta T}{2}\hat{T}}\,\tilde{\varphi}_{>,m}(n_T-1) \tag{4.32}$$

and the same propagation scheme as in (4.23) and (4,24) can be applied for $(n_T-1)I_L+1 \leq i \leq n_T I_L$. Therefore between any two contiguous orthogonalizations of the single particle wave functions (see sect.1) one can compute with this algorithm the forces from $(n_T-1)I_L+1 \leq i \leq n_T I_L$.

It is worth noting that the norm N_{n_T-1} and N_{n_T} do not appear in the forces because they do not depend on each $\sigma_r(i)$ for $(n-1)IL+1 \leq i \leq nIL$.

I hope that the algorithm is now clear.

Firstly one propagates the advanced wave function orthogonalizing any I_L steps and storing in the memory all the single particle wave functions (which at any time give a representation of the many body state) at the time $n_T I_L \Delta T$ (orthogonalized wave function) for $n_T = 1,\ldots,I_P-1$ and at time $(i-1/2)\Delta T, i = 1,\ldots,N_T$. Afterwards one begins the backward propagation of $\varphi_<^{A^{-1}}$ and $\tilde{\varphi}_{<,m}$ by firstly computing the matrix $(A_{m,n})^{-1}$ between any two contiguous orthogonalizations ($\tilde{\varphi}_j^<$ must be also propagated for the calculation of the matrix A at the next orthogonalization). Then the calculation of the forces requires an amount of $I_P(N^2 N_a + N^3)$ operations which save some time if $I_P \ll N_T$.

It is worth noting that the algorithm can be even performed if one could orthogonalize in an adaptive way, i.e. without a fixed value of IL, each time a large fluctuation of σ require a better stability of the algorithm.

Finally we write the explicit expression of the forces using eqs. (4.18–4.26) and taking in mind the discussed propagation scheme

$$F_{r_j}(i) = \sigma_{r_j}(i) + \sqrt{U\Delta T}\left(\sum_k < \varphi_{<,k}^{\uparrow\,A^{-1}}(i)\,|\,\hat{c}_{r_j}^{+\uparrow}\,\hat{c}_{r_j}^{\uparrow}\,|\,\varphi_{>,k}^{\uparrow}(i) >\right)$$

$$-\,,\sqrt{U\Delta T}\left(< \varphi_{<,k}^{\downarrow\,A^{-1}}(i)\,|\,\hat{c}_{r_j}^{+\downarrow}\,\hat{c}_{r_j}^{\downarrow}\,|\,\varphi_{>,k}^{\downarrow}(i) >\right) \tag{4.33}$$

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4.3 Ground state expectation values of operators

In order to have some information from the Langevin dynamic (2.14) and (2.17) about the properties of the Ground state we are interested in the calculation of some observable quantity in terms of time average of classical operators $A(\sigma)$ – called estimators.

The dynamics of σ develops according to the L.E. in which we already knows how to calculate the systematic force (4.33) and the stochastic term app.3 As we have seen, in such calculation, one of the most time consuming operation is the inverse of a matrix A at each time we perform an orthogonalization of the single particle wave functions.

We now show that A^{-1} (spin up and spin down) contains a lot of informations about ground state expectation values of operators of physical interest.

According to the previous section we can compute any observable quantity by a suitable derivative of the free energy

$$F = \lim_{N\to\infty} \frac{1}{N_T} \ln Z$$

Using that $F^+ \longrightarrow F$ (under suitable assumptions) we easily get the answer.

In particular let $\hat{O}$ be any operator, we add to the Hamiltonian $\hat{H}'$ a term $hBhatO$ .Then

$$\left.\frac{\partial}{\partial h}\right|_{h=0} F = \left.\frac{d}{dh}\right|_{h=0} \frac{1}{N_T} \ln < \psi_0 \,|\, e^{-N_T(\hat{H}'\,\Delta T - h\hat{O})} \,|\, \psi_0 > \tag{4.34}$$

The evaluation of such derivative must be done carefully because the operators $\hat{O}$ and $\hat{H}$ do not commute. It is convenient (using essentially the same trick as in Ch.I) to write the full many body propagator as:

$$e^{(\hat{H}'\,\Delta T - h\hat{O})N_T} = \prod_{i=1}^{N_T} \left[e^{+\frac{h}{2}\hat{O}}\, e^{-\Delta T \hat{H}'}\, e^{+\frac{h}{2}\hat{O}} \right] \tag{4.35}$$

up to $o\left((\Delta T)^3, h^2\Delta T, h(\Delta T)^2 h^3\right)$. Hence the calculation is straightforward:

$$\left.\frac{\partial}{\partial h}\right|_{h=0} F = \frac{1}{N_T} \sum_{i=0}^{N_T} g_i \frac{< \psi_0 \,|\, e^{-\hat{H}'\,\Delta T\, i\hat{O}}\, e^{-\hat{H}'\,(NT-i)\,\Delta T} \,|\, \psi_0 >}{< \psi_0 \,|\, e^{-\hat{H}'\,N_T\,\Delta T} \,|\, \psi_0 >} \tag{4.36}$$

$$g_i = \begin{cases} \frac{1}{2} & \text{for } i = 0, N_T \\ 1 & \text{otherwise} \end{cases}$$

When N_T is sufficiently large most of the terms in the preceding sum are using eq. (1.1) nearly equal to:

$$< \psi_G | \hat{O} | \psi_G >$$

apart from the ones which are close to the initial and final time $i \simeq 0$ or N_T. Therefore:

$$\frac{\partial F}{\partial h} = < \psi_G \,|\, \hat{O} \,|\, \psi_G > + o\left(\frac{1}{N_T}\right) \tag{4.37}$$

The convergence can be clearly performed if we add a field $h_i\hat{O}$ where $h_i = h$ for $i \in \{n\}$ far from the initial and the final time (i.e. $i \simeq N_T$ or 0) and $h_i = 0$ otherwise. The important thing is that the field h_i must be different from 0 at least in a number of time steps I_P which is a fixed factor of $N_T = I_L I_P$. Even in this case, in fact

$$\frac{\partial F}{\partial h} = \frac{1}{IL} < \psi_G \,|\, \hat{O} \,|\, \psi_G > \qquad for\, N_T \longrightarrow \infty \tag{4.38}$$

After the H.S.T. is performed all the calculation can be done if one knows for any n the following quantity:

$$\frac{< \psi_0 \,|\, \prod_{m=n}^{N_T} \hat{U}_{\sigma(m)}\, \hat{O} \prod_{m=1}^{n-1} \hat{U}_{\sigma(m)} \,|\, \psi_0 >}{< \psi_0 \,|\, \hat{U}_\sigma \,|\, \psi_0 >} = A^n_{\hat{O}}(\sigma) \tag{4.39}$$

from which using (4.38) and $N_T = I_P I_L$,

$$< \psi_G \,|\, \hat{O} \,|\, \psi_G > = \frac{1}{I_P} \sum_{k=\{n\}} < A^k(\sigma) > \qquad for\, I_P \longrightarrow \infty \tag{4.40}$$

Hence the calculation of the ground state expectation value $< \psi_G|\hat{O}|\psi_G >$ as a derivative of the free energy (4.34) can be achieved with the statistical average of I_P different quantities (with $I_P < N_T$). As we will see later such calculation requires about the same amount of computer time needed for the forces (5.16) at least for operators $\hat{O}$ which are contractions of the 2 and 4–point Green functions. On the other hand the statistical error corresponding to:

$$\frac{1}{I_P} \sum_{k=\{n\}} A^k(\sigma)$$

is about $\frac{1}{\sqrt{I_P}}$ less than the one of a single $A^n(\sigma)$. Moreover using the fact that free energy F is presumably equal to F^+ (see eq.3.13), one can take the advantage to sample only the positive $< \psi_0|\hat{U}_\sigma|\psi_0 >$ region.

Due to th e discrete Langevin time the σ–configuration can jump from a positive $< \psi_0|\hat{U}_\sigma|\psi_0 >$ region to a negative one (and viceversa). Hereafter the potential is assumed to be V in (2.7) and the averages limited to the positive or negative $< \psi_0|\hat{U}_\sigma|\psi_0 >$ region.The estimators corresponding to a general operator is calculated using the statistical method described in Ch.2 sect.2 and according to eq.(3.7) we independently update the averages over the positive and negative $< \psi_0|\hat{U}_\sigma|\psi_0 >$ region.

4.4 Evaluation of the four-point equal-time Green's function

Let us consider the 4-point equal-time Green's function:

$$< \psi_G \mid \hat{c}_j^{\alpha} \hat{c}_j^{\beta} \hat{c}_{\kappa}^{+^{\delta}} \hat{c}_l^{+^{\gamma}} \mid \psi_G > \tag{4.41}$$

In the following $c_i^{+^{\alpha}}$ ($\alpha = \uparrow$ or $\downarrow$) are creation operators of a particle in a state with defined space coordinate and spin projection. After repeating the same steps as in the preceding section with

$$\hat{O} = \hat{c}_j^{\alpha} \hat{c}_j^{\beta} \hat{c}_{\kappa}^{+^{\delta}} \hat{c}_l^{+^{\gamma}} \tag{4.42}$$

we need in general the calculation of $A_{\hat{O}}^n(\sigma)$ that for such operator $\hat{O}$ – using a single particle determinant trial function – is proportional to the scalar product of two Slater determinants with $M+2$ particles. In fact

$$A_{\hat{O}}^n(\sigma) = \frac{< \hat{c}_j^{+^{\beta}} \hat{c}_i^{+^{\alpha}} \prod_{m=N_T}^{n} \hat{U}_{\sigma(m)} \psi_0 \mid \hat{c}_k^{+^{\delta}} \hat{c}_l^{+^{\gamma}} \prod_{m=1}^{n-1} \hat{U}_{\sigma(m)} \psi_0 >}{< \prod_{m=N_T}^{n} \hat{U}_{\sigma(m)} \psi_0 \mid \prod_{m=1}^{n-1} \hat{U}_{\sigma(m)} \psi_0 >} \tag{4.43}$$

where for convenience we have rewritten the denominator of (4.39) in a slightly different way.

Using the definition of the forward and backward propagated wave function $\tilde{\varphi}^{<}$ and $\tilde{\varphi}^{>}$ (4.31) (where for convenience we don't write the subindex $n = mI_L - 1$), one can write the previous expression by using the straightforward formula which gives the scalar product of two Slater determinants in (4.43). If $\alpha, \gamma = \uparrow$ and $\beta, \delta = \downarrow$ and symmetric permutations:

$$A_{\hat{O}}(\sigma) = \frac{det\, \underline{A}^{\uparrow}(i,l)\, det\, \underline{A}^{\downarrow}(j,k)}{det\, A^{\uparrow}\, det\, A^{\downarrow}} \tag{4.44}$$

where $\underline{A}$ ($\uparrow$ or $\downarrow$) is a matrix $(M+1) \times (M+1)$ (for any (i,l) or (j,k)) indexed by the single particle wave function components (with $\uparrow$ or $\downarrow$ spin projection)

$$\underline{A}_{m,n}(j,k) = \begin{pmatrix} \delta_{j,k} & \tilde{\varphi}_n^{>}(r_k) \\ \tilde{\varphi}_m^{<}(r_j) & A_{m,n} \end{pmatrix} \tag{4.45}$$

and $A_{m,n}$ is a matrix $M \times M$

$$A_{m,n} = < \tilde{\varphi}_m^{<} | \tilde{\varphi}_n^{>} >$$

On the other hand when $\alpha = \beta = \gamma = \delta = \uparrow$ (or $\downarrow$)

$$A^n_{\hat{O}}(\sigma) = \frac{det\, \underline{A}^{\uparrow}}{det\, A^{\uparrow}} \tag{4.46}$$

where $\underline{A}$ ($\uparrow$ or $\downarrow$) is now a matrix $(M+2)\times(M+2)$ for any i,l,j,k, indexed by the single particle wave function components (with $\uparrow$ or $\downarrow$ spin projection)

$$\underline{A}_{m,n}(i,j,k,l) = \begin{pmatrix} \delta_{k,j} & \delta_{i,k} & \tilde{\varphi}^{>}_n(r_k) & \cdots \\ \delta_{j,l} & \delta_{i,l} & \tilde{\varphi}^{>}_n(r_l) & \cdots \\ \tilde{\varphi}^{<}_m(r_j) & \tilde{\varphi}^{<}_m(r_i) & & \\ \vdots & \vdots & A_{m,n} & \end{pmatrix} \tag{4.47}$$

From expressions (4.45) and (4.47) the calculation of the Green's function requires at least the evaluation of two determinants for any fixed i,j,k,l.

However several interesting operators like:

$$S_M(q) = \frac{1}{N_a}\sum_{i,j} e^{-iq(r_i-r_j)} < \psi_G \,|\, \hat{m}_{r_i}\, \hat{m}_{r_j} \,|\, \psi_G > \tag{4.48}$$

$$S(q) = \frac{1}{N_a}\sum_{i,j} e^{-iq(r_i-r_j)} < \psi_G \,|\, \hat{n}_{r_i}\, \hat{n}_{r_j} \,|\, \psi_G > \tag{4.49}$$

with $\hat{n}_{r_i} = \hat{c}^{+\uparrow}_{r_i}\,\hat{c}^{\uparrow}_{r_i} + \hat{c}^{+\downarrow}_{r_i}\,\hat{c}^{\downarrow}_{r_i}$

$$S_{BCS}(\tau,q) = \frac{1}{N_a}\sum_{i,j} e^{-iq(r_i-r_j)} < \psi_G \,|\, \hat{c}^{\downarrow}_{j+\tau}\,\hat{c}^{\uparrow}_{j}\,\hat{c}^{+\uparrow}_{i}\,\hat{c}^{+\downarrow}_{i+\tau} \,|\, \psi_G > \tag{4.50}$$

requires the calculation of the Green's function for N^2 different values and results in a considerable waste of time.

It is worth mentioning that the previous ground state expecta tion values (eqs.4.48-4.50) allows to characterize many interesting physical properties of the quantum system. In particular the correlation function S_{BCS} is useful to investigate , as shown by Hirsch (1987), the superconducting property of the ground state; the remaining ones give informations about the density (S) and magnetic (S_M) fluctuations.

In order to improve the algorithm we simply note that the considered N_a^2 matrices, (4.45) and (4.47), differ one from the other (for different values of i,j,k,l) only for few rows or columns. It is possible to simplify the problem and formulate all the calculation in terms of the quantities:

$$B(j,k) = \sum_{m,n} \tilde{\varphi}^{>}_m(r_k)\, A^{-1}_{m,n}\, \tilde{\varphi}^{<}_n(r_j) \tag{4.51}$$

In fact the determinant of $\underline{A}$ ($\uparrow$ or $\downarrow$) in case $\alpha \neq \beta$ can be written using the well known properties of the determinants (the determinant of a matrix $\underline{A}$ remains unchanged by adding to a column – first one – any linear combination of other columns chosen in particular to make vanishing all the first column elements but the one in the first row):

$$det \begin{pmatrix} 1-\delta_{j,k} & \tilde{\varphi}^{>}_{n}(r_k) \\ \tilde{\varphi}^{<}_{m}(r_j) & A_{m,n} \end{pmatrix} = det \begin{pmatrix} \delta_{j,k} - \sum\limits_{n} c_n \, \tilde{\varphi}^{>}_{n}(r_k) & \tilde{\varphi}^{>}_{n}(r_k) \\ \tilde{\varphi}^{<}_{m}(r_j) - \sum\limits_{n} A_{m,n} \, c_n & A_{m,n} \end{pmatrix} \tag{4.52}$$

where in order to have:

$$\tilde{\varphi}^{<}_{m}(r_j) - \sum_{n} A_{m,n} \, c_n = 0 \tag{4.53}$$

one has to take:

$$c_m = \sum_{n} A^{-1}_{m,n} \, \tilde{\varphi}^{<}_{n}(r_j) \tag{4.54}$$

substituting the last expression in the R.H.S. of (4.52) and using the definition (4.51) one gets:

$$det \begin{pmatrix} \delta_{j,k} & \tilde{\varphi}^{>}_{n}(r_k) \\ \tilde{\varphi}^{<}_{m}(r_j) & A_{m,n} \end{pmatrix} = \begin{pmatrix} \delta_{j,k} - B(j,k) & \tilde{\varphi}^{>}_{n}(r_k) \\ 0 & \\ 0 & \\ 0 & A_{l,m} \\ \vdots & \end{pmatrix} = det\, A \; (\delta_{j,k} - B(j,k)) \tag{4.55}$$

In the calculation of $A_{\hat{O}}(\sigma)$ in (4.44) the factor $detA$ cancels out with the denominator:

$$A_{\hat{O}}(\sigma) = [\delta_{j,k} - B(j,k)] \, [\delta_{i,l} - B(i,l)] \tag{4.56}$$

If $\alpha = \beta = \uparrow$ (or $\downarrow$), after cumbersome algebra, repeating the same trick as before (i.e. by zeroing all the elements of the first two columns of $\underline{A}$ except the ones in the first two rows, and then by using the Lagrange expansion of a determinant) one obtain:

$$det\, \underline{A}_{m,n} = \begin{pmatrix} \delta_{k,j} - B(j,k) & \delta_{i,k} - B(i,k) & \tilde{\varphi}^{>}_{n}(r_k) & \cdots \\ \delta_{j,l} - B(j,l) & \delta_{i,l} - B(i,l) & \tilde{\varphi}^{>}_{n}(r_l) & \cdots \\ 0 & 0 & & \\ 0 & 0 & A_{m,n} & \\ \vdots & \vdots & & \end{pmatrix}$$

$$= [\delta_{j,k} - B(j,k)][\delta_{i,l} - B(i,l)] - [\delta_{i,k} - B(i,k)][\delta_{j,l} - B(j,l)]\, det\, A \tag{4.57}$$

Hence using (4.46)

$$A_{\hat{O}}(\sigma) = [\delta_{j,k} - B(j,k)][\delta_{i,l} - B(i,l)] - [\delta_{i,k} - B(i,k)][\delta_{j,l} - B(j,l)] \qquad (4.58)$$

The last expression is exactly the 2×2 determinant in the top left side of the previous large matrix in (4.57).

Hence the ground state expectation value of any operator $\hat{O}$ which derive from a suitable contraction of the 4-point equal-time Green's function (4.41) can be obtained from the statistical thermal average of a classical operator $A_{\hat{O}}/\sigma)$ (estimator of the operator $\hat{O}$) expressed in terms of the elements of two $N_a \times N_a$ square matrices $B^{\uparrow}$ and $B^{\downarrow}$ (4.51).

Of course the two point equal-time Green's function:

$$< \psi_G \,|\, \hat{c}_i^{\alpha}\, \hat{c}_j^{+^{\alpha}} \,|\, \psi_G > \qquad (4.59)$$

can even be expressed in terms of $B(i,j)$. In fact, following the same steps as in the previous case:

$$A_{\hat{c}_i^{\alpha}\, \hat{c}_j^{+\alpha}}(\sigma) = \delta_{i,j} - B^{\alpha}(i,j) \qquad (4.60)$$

and the estimator of any one–body operator can be easily written in terms of $B^{\uparrow}$ and $B^{\downarrow}$.

The basic operation for the calculation (5.35) of all the elements of the matrices $B^{\uparrow}$ and $B^{\downarrow}$ is the inversion of two $N \times N$ matrices $A^{\uparrow}$ and $A^{\downarrow}$ (N^3 operations), a change of basis $A^{-1}\tilde{\varphi}^{<}$ ($N^2 N_a$ operations) and remaining N multiplications for each different couple of lattice sites (N_a^2) for which the matrices $B^{\alpha}(i,j)$ are defined. In this way the computation time required for updating the matrices B^{α} takes less than $o(N_a^3)$ operations. As we shall see the estimators of any static structure factor defined in (4.48-4.50) takes N_a^2 operations for each different q , once the values of $B^{\alpha}(i,j)$ are known.

At this point it is worth mentioning that the estimator $A_{\hat{O}}(\sigma)$ in expressions (4.44) and (4.46) does not depend on the norms of the propagated many body wave function (the numerator factor cancels with the denominator one) and of course on the one particle orbitals chosen for the representation of the given Slater determinant. Hence it is convenient to calculate $A_{\hat{O}}^{n}(\sigma)$ for each n in which one performs an orthogonalization because the matrix A^{-1} needed for such operation (see sect.1) can be even used for the calculation of $B(i,j)$.

Finally let us summarize the explicit expressions for the three considered quantities (4.48-4.50) in terms of B^{α}. They can be obtained ,after a straightforward and cumbersome algebra, using equation (4.56-4.58) and the canonical commutation rules for the $\hat{c}_i, \hat{c}_j$ in the expression of the 2 and 4–point Green's function (4.60) and (4.41)

$$A_{S(q)}(\sigma) = \frac{1}{N_a}\sum_{k,j} e^{-iq(r_k-r_j)}\left[B^{\uparrow}_{r_k,r_k}B^{\uparrow}_{r_j,r_j} - B^{\uparrow}_{r_k,r_j}B^{\uparrow}_{r_j,r_k} + B^{\uparrow}_{r_k,r_k}B^{\downarrow}_{r_j,r_j} + \delta_{k,j}B^{\uparrow}_{r_k,r_j} + \uparrow\rightleftharpoons\downarrow\right]$$

$$A_{S_M(q)}(\sigma) = \frac{1}{N_a}\sum_{k,j} e^{-iq(r_k-r_j)}\left[B^{\uparrow}_{r_k,r_k}B^{\uparrow}_{r_j,r_j} - B^{\uparrow}_{r_k,r_j}B^{\uparrow}_{r_j,r_k} - B^{\uparrow}_{r_k,r_k}B^{\downarrow}_{r_j,r_j} + \delta_{k,j}B^{\uparrow}_{r_k,r_j} + \uparrow\rightleftharpoons\downarrow\right]$$

$$A_{S_{BCS}(q)} = \frac{1}{N_a}\sum_{r_k,r_j}\left[(\delta_{k,j} - B^{\uparrow}_{r_k,r_j})(\delta_{k,j} - B^{\downarrow}_{r_j+\underline{\tau},r_k+\underline{\tau}})\right] e^{-iq(r_k-r_j)} \qquad (4.61)$$

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4.5 Calculation of the ground state energy

In addition to expression (1.24) one can calculate the ground state energy by a suitable contraction of the two and four point Green's functions. In this case the correspondent classical operators for the energy is from eqs.(1.11) (4.56) and (4.60).

$$A^n_E(\sigma) = T\sum_{<i,j>} B^{\uparrow}_{r_i,r_j} + B^{\downarrow}_{r_i,r_j} + U\sum_i B^{\uparrow}_{r_i,r_i}B^{\downarrow}_{r_i,r_i} \qquad (4.62)$$

Actually the first term in the R.M.S. of the preceding equation gives the average kinetic energy while the second one the average potential energy.

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4.6 Conjugate variables

In chapter we performed an H.S.T. using the Ising scheme. In this scheme the σ_{r_j} variables for a given site r_j are conjugate to the local magnetization operator $\hat{m}_{r_j}$ in the same site. To see why (suppose N_T fixed) we add an infinitesimal field $h_r(i)$ linearly coupled to the local magnetization operator in the Hamiltonian $\hat{H}$ so that the partition function (3.1) reads up to $o(h(\Delta T)^2)$:

$$Z = <\psi_0|\prod_{i=0}^{N_T} e^{-\hat{T}\frac{\Delta T}{2}}\, e^{-V\Delta T + \sum_r h_r(i)\hat{m}_r}\, e^{-\frac{\Delta T}{2}\hat{T}}|\psi_0> \qquad (4,63)$$

After using the H.S.T. the single particle operator $\hat{U}_\sigma$ in (1.15) become now:

$$\hat{U}_\sigma = \prod_{i=1}^{N_T} e^{-\frac{\Delta T}{2}\hat{T}}\, e^{-\sqrt{U\Delta T}\sum\sigma_r(i) + h_r(i)\hat{m}_r}\, e^{-\frac{\Delta T}{2}\hat{T}} \qquad (4.64)$$

This means that after the change of variables

$$\sigma'_r(i) = \sigma_r(i) + \frac{h_r(i)}{\sqrt{U\,\Delta T}} \qquad [d\sigma'] = [d\sigma] \tag{4.65}$$

the dependence of $\hat{U}_\sigma$ from the field $h_r(i)$ disappears. Therefore Z reads:

$$Z = \int [d\sigma']\, e^{-\frac{1}{2}\sum_{r,i}\left[\sigma'_r(i) - \frac{h_r(i)}{\sqrt{U\,\Delta T}}\right]^2} < \psi_0 \,|\, \hat{U}_{\sigma'} \,|\, \psi_0 > \tag{4.66}$$

By differentiating expression (4.64) and (4.66) with respect to $h_r(i)$ one easily gets relations between ground state average of operators containing $\hat{m}_r$ and corresponding classical averages of the conjugate variables σ_r (over the potential $V(\sigma)$ in the positive and negative $< \psi_0|\hat{U}_\sigma|\psi_0 >$ region). In particular (all the static and imaginary time dynamical correlation function are easily obtained) the magnetic correlation function:

$$\begin{aligned} < \psi_G \,|\, \hat{m}_{r_i}\, \hat{m}_{r_j} \,|\, \psi_G > &= \lim_{N_T \to \infty} \frac{\dfrac{\partial^2 Z}{\partial h_r(N_T/2)\, \partial h_r(N_T/2)}}{Z} \\ &= \frac{1}{U\,\Delta T}\left[< \sigma_{r_i}\left(\frac{N_T}{2}\right) \sigma_{r_j}\left(\frac{N_T}{2}\right) > - \delta_{r_i, r_j} \right] \end{aligned} \tag{4.67}$$

The latter equation also shows that the on-site fluctuations of σ are larger $(< \psi_G|\hat{m}_r^2|\psi_G > \geq 0)$ than the corresponding gaussian fluctuations $(< \sigma_r^2 >= 1)$. In this sense the method is not very convenient for quantities which depend on the same site σ_r–correlation. Actually we obtained a better statistical error by computing such quantities (like energy, $S_M(q)$ etc.) with the direct evaluation of the Green's functions (method b) i.e. without the change of variables (4.65) before differentiating Z.

CHAPTER V

Testing the algorithm

In this chapter we present some numerical calculations we made using the algorithm described in the preceding sections for the 1D-system of fermions coupled by a short range positive interaction term. Before considering all the results it is worth mentioning that the algorithm was tested using non optimal trial functions and large number of variables. This was done in order to check the numerical stability and show the advantage of the orthogonalization scheme (Ch.IV).

The half–filled 1D Hubbard–model was exactly solved by Lieb and Wu (1969). It turned out that the ground state of the Hamiltonian shows a tendency of antiferromagnetism for any $U > 0$ (without long range order). Thus we choose as a test function $|\psi_0>$ the simple paramagnetic one which is made up by single particle real plane wave functions ($\sin kr_i$ or $\cos kr_i$) with $N/2$ spin up and $N/2$ spin down. This many–body wave function gives the exact ground state of the Hamiltonian for $U = 0$. Therefore we tested the algorithm for large U. In fig.1 it is shown a typical Langevin dynamics evolution of the instantaneous ground state energy. Such instantaneous energy converges very fastly close to the exact value (the central line drawn in the fig.1). In figs.2–6 we analyse the size dependence of the Ground state energy and the static structure factors as defined in (4.48–4.50). The exact results for the energy were taken from ref.5,8 and in this case we used a first order Langevin algorithm eq.(2.19).

Although the computation time required for small systems was relatively large it was really surprising that the algorithm gave reasonable results under such bad conditions (he importance sampling depend on the chosen test function). Moreover the algorithm showed to be very stable even for large N_T that is very small effective temperature ($kT \simeq \frac{1}{NT\Delta T} \simeq 10$ times less then the minimum temperature reached by Hirsch). Numerical results are reported for two different effective temperatures. Apart for the very encouraging quantitative calculations of the ground state energy we can also see that the qualitative behaviour of $S_M(\pi)$ is reasonable because it shows an enhanced antiferromagnetism. In fact $S_M(\pi)$ is considerably larger than the corresponding $S_{BCS}(0)$ (see fig.3, 6) correlation function (such function is used to describe the Cooper-pair correlations). However the very large difference between the results at the two different effective temperatures shows that the convergence with respect to temperature has not

reached yet. To better display this feature we fixed $U = 4$ in an 8–site Hubbard ring (eq.1.1) and we made calculations for several values of N_T. The convergence of $S_M(\pi)$ is reached after twice the time ($NT\Delta T$) needed for the ground state energy (fig.13) and the other correlation functions (fig.14-16).

As shown in Ch.III eq.5.12 the convergence of F^+ behaves like $!/NT$ (if $r \neq 0$) while the convergence of F is exponential in time $NT\Delta T$.

Let us call from now on the error due to a finite NT, the systematic error. As mentioned in sect.4.3, the statistical error which derive from any estimator decrease like the inverse square root of N_T. Therefore it is clear that when N_T is very large the systematic error become negligible with respect to the statistical one.

It is not possible to understand with the available data if the convergence is exponential or follows a power low. On the other hand we found configurations with negative determinant as frequent as the positive determinant ones, even for very large N_T.

The ground state energy has shown to be a monotonic function of U , this is in agreement with the results drawn in fig.7.

In figs.12,14,16 it is also shown that the averages on the positive determinant region coincide within the statistical error with the negative determinant averages provided N_T is large enough.

As a further test of the reliability of the algorithm, we calculated $S_M(q)$ and the static spin susceptibility χ_{st}. It is easy to show that:

$$\chi_{st} = S_M(q = 0) = 0$$

In fact $S_M(q = 0)$ (an analogous argument holds for χ_{st}) can be written as:

$$S_M(q = 0) = \frac{1}{N_a} < \psi_G \mid \hat{M}^2 \mid \psi_G >$$

and $S_M(q = 0) = 0$ is a consequence of $\hat{M}\psi_G = 0$ for the 1D ground state. The results (figs.4,7) are consistent within the statistical error.

In the last figs.13,15 we made a comparison between the two methods (a) and (b) used for the calculation of the energy. The method (a) is calculated by a numerical estimation of the derivative in eq.1.24 for a fixed configurations σ, while the method (b) follows from the direct evaluation of the Green's function (eq.4.62).

Similarly the magnetic structure factor is calculated either by means of the conjugate variables or as for the energy with the 2 and 4-point Green's function

Method (a): using the conjugate variables.(eq.467)

Method (b): eq. (4.51)

In both cases the estimators of E and $S_M(\pi)$ by means of the 2 and 4–point static Green function produce smaller statistical error than the ones related obtained with the method (a). The reason of this has already been explained in the previous sections.

CHAPTER VI

Conclusions and perspectives for the future

In the last few months remarkable attention have been devoted to the study of the 2D Hubbard model in order to understand a possible superconductive behaviour of the ground state for large positive U, close to the half–filled density $N \leq N_a$.

In this sense it is interesting to study the BCS correlation functions defined in eq.(4.50). If there is a superconductive phase the expectation values of operators $\hat{O} = \sum_i \hat{c}_i^{+\uparrow}\, \hat{c}_{i+\tau}^{+\downarrow}$:

$$\frac{1}{N_a} < \hat{O} >$$

must be finite for $N_a \longrightarrow \infty$ (if $\tau = 0$, $\frac{1}{N_a} < \hat{O} >$ is proportional to the gap in the ordinary B.C.S. theory).

However with the present method we cannot measure non–zero values of $< \hat{O} >$ because we can only deal with a system with a fixed number of particles. Therefore it would be impossible to characterize a superconductive phase by examining the expectation value of $\hat{O}$ without adding a breaking symmetry term in the Hamiltonian ($h\hat{O}$ as an example) which in this case makes the problem prohibitive.

On the other hand, consider the expectation value of:

$$\frac{1}{N_a} < \psi_G \,|\, \hat{O}^+ \hat{O} \,|\, \psi_G > = S_{BCS}(0) \quad see\ eq.4.50$$

The latter quantity is different from zero even for finite N_a and $h = 0$ because the operator $\hat{O}\hat{O}^+$ commutes with the particle number operator and is invariant under phase rotation symmetry ($\hat{c}_i \rightarrow e^{i\theta}\hat{c}_i$) which is broken in the superconductive state. Hence for each h and N_a one has:

$$\left| < \psi_G \,|\, \hat{O} \,|\, \psi_G > \right| \leq < \hat{O}\,\psi_G \,|\, \hat{O}\,\psi_G >^{\frac{1}{2}}$$

from the Schwartz inequality. Thus

$$\left[\frac{1}{N_a} < \psi_G \,|\, \hat{O} \,|\, \psi_G > \right]^2 N_a \leq \frac{1}{N_a} < \psi_G \,|\, \hat{O}^+ \hat{O} \,|\, \psi_G >$$

Supposing that the R.H.S. in the previous inequality does not depend strongly on h (the two limits $N_a \rightarrow \infty, h \rightarrow 0$ can be interchanged for symmetric operator) then it easily follows

that whenever a spontaneous breaking phenomena occurs ($\frac{1}{N_a} < \psi_G | \hat{O}^+ \hat{O} | \psi_G > \neq 0, for N_a \to \infty$). Then the expectation value of

$$\frac{1}{N_a} < \psi_G | \hat{O}^+ \hat{O} | \psi_G >_{h=0}$$

grows at least as the size of the system. In this way our method can be applied even for studying a possible superconductive phase in the 2D Hubbard model. In my opinion the latter possibility is one of the most interesting application of the present method provided 200–300 hours of Cray can be used. Further application of this nethod may be found in the electronic structure problem. In fact the LDA calculations, which nowadays can be even performed for relatively large systems (Car and Parrinello 1985), can be used ,in a very natural way, as a starting point of the present method ($|\psi_0 >$ made up by the one particle orbitals deriving from the LDA).

APPENDIX 1

a)

Consider the matrix $\hat{U}$ for a fixed NT:

$$\hat{U} = \int [d\sigma]\, e^{-\frac{1}{2}\underline{\sigma}^2 \hat{U}_\sigma} < \psi_0 \,|\, \hat{U}_\sigma \,|\, \psi_0 \geq 0 \tag{A1.1}$$

then: $\hat{U} = \hat{U}^+$.

It is sufficient to note that after the operation of <u>time-reversal</u>

$$\sigma(1), \sigma(2), \cdots, \sigma(NT) \rightarrow \sigma'(NT), \sigma'(NT-1), \cdots, \sigma'(1)$$

the σ' satisfying $< \psi_0 | \hat{U}_\sigma | \psi_0 > \geq 0$ remains in the same ensemble. In fact after the latter transformation $\hat{U}_\sigma \longrightarrow \hat{U}_\sigma^+$ and if $< \psi_0 | \hat{U}_\sigma | \psi_0 > \geq 0$ then $< \psi_0 | \hat{U}_\sigma^+ | \psi_0 > \geq 0$ again (and viceversa). Therefore:

$$\hat{U} = \hat{U}^+ \tag{A1.2}$$

////

b)

$$\frac{Z_+^2(k)}{Z_+(k+1)} \leq 1 \tag{A1.3}$$

In fact consider:

$$Z_+^2(k) \leq Z_+^2(k) + \sum_{i=1}^{D} Z_i^2(k) \tag{A1.4}$$

where:

$$\begin{aligned} Z_i(k) &= \int_{<\psi_0|\hat{U}_\sigma|\psi_0> > 0} [d\sigma]\, e^{-\frac{1}{2}\underline{\sigma}^2 <\psi_0|\hat{U}_\sigma|\psi_i>} \\ &= < \psi_0 | \hat{U} | \psi_i > \quad (from\,(a)\, because\, \hat{U} = \hat{U}^+) \\ &= < \psi_i | \hat{U} | \psi_0 > \\ &= \int [d\sigma]\, e^{-\frac{1}{2}\underline{\sigma}^2} < \psi_i \,|\, \hat{U}_\sigma \,|\, \psi_0 > \end{aligned} \tag{A1.5}$$

and $|\psi_0>$ $\{|\psi_i>\}$ is a complete set in the given $(D+1$ dimensional Hilbert space. Therefore:

$$Z_+^2 + \sum_{i=1}^{D} Z_i^2(k) = \int_{D_\sigma} [d\sigma_1]\,[d\sigma_2]\, e^{-\frac{1}{2}(\sigma_1^2+\sigma_2^2)} \sum_{i=0}^{D} <\psi_0\,|\,\hat{U}_{\sigma_1}\,|\,\psi_i><\psi_i\,|\,\hat{U}_{\sigma_2}\,|\,\psi_0>$$

$$= \int_{D_\sigma} [d\sigma]\, e^{-\frac{1}{2}\sigma^2} <\psi_0\,|\,\hat{U}_\sigma\,|\,\psi_0> \qquad \text{(A1.6)}$$

where the domain of integration D_σ is defined by:

$$<\psi_0|\hat{U}_{\sigma_1}|\psi_0> \geq 0 and <\psi_0|\hat{U}_{\sigma_2}|\psi_0> \geq 0$$

Now $Z_+(k+1)$ from definition (3.6) is the integral of the same function (with $2^{k+1}N_a$ variables) as in (A1.6)

$$e^{-\frac{\sigma^2}{2}} <\psi_0\,|\,\hat{U}_\sigma\,|\,\psi_0> \qquad \text{(A1.7)}$$

but the integral is extended over all the region in which the function itself (A1.7) is positive. Hence from (A1.6):

$$Z_+^2(k) = \sum Z_i^2(k) \leq Z_+(k+1) \qquad \text{(A1.8)}$$

Finally putting together the inequalities (A1.4) and (A1.7)

$$Z_+^2(k) \leq Z_+^2(k) + \sum Z_i^2(k) \leq Z_+(k+1)$$

one obtains the desired result (A1.3).

c)

The absolute maximum of

$$e^{-V(\sigma)} = e^{-\frac{1}{2}\sigma^2} <\psi_0\,|\,\hat{U}_\sigma\,|\,\psi_0> \qquad \text{(A1.9)}$$

and

$$e^{-V(\sigma)} = e^{-\frac{1}{2}\sigma^2} \left\| \hat{U}_\sigma\,|\,\psi_0> \right\| \qquad \text{(A1.10)}$$

coincide if $|\psi_0>$ is the ground state eigenvector of the Hartree solution, where $\sigma(r,i)$ is independent of time i at this maximum.

The Hartree solution is defined in the following self

consistent way:

$$\sigma(r_j,i) = \frac{<\psi_0 \mid A_i^+(\sigma)\,\hat{m}(r_j)\,A_i(\sigma) \mid \psi_0>}{<\psi_0 \mid A_i^+(\sigma)\,A_i(\sigma) \mid \psi_0>}(U\,\Delta T)^{\frac{1}{2}} \qquad \text{(A1.11)}$$

and $|\psi_0>$ is determined to be an eigenvector of A^+A:

$$A^+A|\psi_0>=E|\psi_0>$$

(E is chosen to be the maximum for all possible solution of A1.11) and

$$A_i(\sigma) = e^{-\frac{(U\Delta T)^{\frac{1}{2}}}{2}\sum_j \hat{m}_{r_j}\,\sigma_{r_j}}\; e^{-\hat{T}\frac{\Delta T}{2}} \qquad \text{(A1.12)}$$

($|\psi_0>$ and E does not depend on i).

PROOF:

$$e^{-V(\sigma)} \leq e^{-V'(\sigma)}$$

is a consequence of the Schwartz inequality. But $e^{-V'(\sigma)}$ can be written as:

$$e^{-V'(\sigma)} = \prod_{i=1}^{NT} \hat{B}(\sigma,i) \mid \psi_0>$$

where

$$\hat{B}(\sigma,i) = e^{-\frac{1}{2}\sum_j \sigma^2(r_j,i)\,A_i^+(\sigma)\,A(\sigma)} \qquad \text{(A1.13)}$$

$B^+ = B$ is evident. Then we can use in an iterative way the following property, valid for any symmetric operator and any state $|\Phi>$:

$$\max \| \hat{B}(\sigma,i) \mid \psi> \| \leq \max_k \{\lambda_\kappa(\iota)\}\, \| \mid \psi> \mid \| \qquad \text{(A1.14)}$$

where λ_k are all the eigenvalues of the matrix $B(\sigma,i)$ for fixed i and configuration σ. Therefore:

$$e^{-V'(\sigma)} \leq \prod_{i=1}^{NT} \max_\sigma \max_k \{\lambda_k(i)\} \qquad \text{(A1.15)}$$

But the maximization of any factor of the product give an Hartree solution (A1.11) which is evidently independent of i. Therefore for this state $|\psi_0>$ and this eigenvector $E \geq 0$ ($B(\sigma, i)$ is always positive definite)

$$e^{-V'(\sigma)} \leq E^{NT} \tag{A1.16}$$

and for such $\sigma_r(i)$ independent of i

$$e^{-V(\sigma)} = e^{-V'(\sigma)} = E^{NT} \tag{A1.17}$$

Therefore from the two previous equations, the absolute maximum both of $e^{-V(\sigma)}$ and $e^{-V'(\sigma)}$ coincide for a $\sigma(r, i)$ independent of i.

APPENDIX 2

$F^+(k)$ is bounded by a function independent of k.

In fact:

$$Z_+(k) \leq \int_{all\ space} [d\sigma]\, e^{-\frac{1}{2}\underline{\sigma}^2} \left\| \hat{U}_\sigma \,|\, \psi_0 > \right\|$$

$$\leq e^{-\Delta T\, E_T\, NT} \left[\int \frac{d\sigma}{2\pi}\, e^{-\frac{1}{2}\underline{\sigma}^2 + N(U\Delta T)^{\frac{1}{2}}} \right]^{NT\, N_a} \tag{A2.1}$$

We have used in an iterative way:

$$\max \| A\, \Phi \| \leq \max_i \{ \lambda_i \} \tag{A2.2}$$

When λ_i are all the eigenvalues of A (symmetric matrix) and for

$$e^{-\frac{\Delta T}{2}\hat{T}} \longrightarrow \max \lambda_i = e^{-E_T \frac{\Delta T}{2}} \tag{A2.3}$$

where E_T is the ground state energy of the kinetic operator in the considered Hilbert space.

$$e^{-\sum_r \sigma(i,\underline{r})(n^\uparrow - n^\downarrow)\sqrt{U\Delta T}} \longrightarrow \max \lambda_i \leq e^{+\sum_r |\sigma(i,r)|\sqrt{U\Delta T}} \tag{A2.4}$$

Using the fact that the eigenvalues of $n^\uparrow$, $n^{downarrow}$ are 1 or 0. But

$$\int_{-\infty}^{+\infty} \frac{d\sigma}{2\pi}\, e^{-\frac{1}{2}\underline{\sigma}^2 + N\sqrt{U\Delta T}}$$

$$= 2 \int_0^{\infty} \frac{d\sigma}{2\pi}\, e^{-\frac{1}{2}\underline{\sigma}^2 + N\sqrt{U\Delta T}}$$

$$\leq 2 \int_{-\infty}^{+\infty} \frac{d\sigma}{2\pi}\, e^{-\frac{1}{2}\underline{\sigma}^2\, U\Delta T\, N^2}$$

$$= e^{U\Delta T\, N^2 + \ln\sqrt{\pi}} \tag{A2.5}$$

Then

$$Z_+(k) \leq e^{NT\left[-E_T\Delta T + N^2\, U\, \Delta T\, N_a + \frac{N_a}{2}\ln\pi\right]} \tag{A2.6}$$

and finally:

$$F^+(k) \leq -E_T\,\Delta T + N_a\, N^2\, U\, \Delta T + \frac{1}{2}\ln(\pi)\, N_a \tag{A2.7}$$

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REMARK

From (A1.3) $F^+(k+1) \geq F^+(k)$, therefore from (A2.7)

$$\lim_{k \to \infty} F^+(k)$$

exists and is finite. F^+ is then a well defined free energy.

APPENDIX 3: THE H.S.T. FOR A GENERAL FERMIONIC OPERATOR

Consider a general interaction term :

$$\sum_{i,j} v_{i,j}\, \hat{n}_i\, \hat{n}_j \tag{A.3.1}$$

where $\hat{n}_i$ is the density operator of a fermion at a given site and for a defined spin projection. Then, using that $\hat{n}_i^2 = \hat{n}_i$ for a Fermi-operator one can write:

$$\sum_{i,j} v_{i,j}\, \hat{n}_i\, \hat{n}_j \;=\; \sum_{i,j} \left[v_{i,j} \;-\; \lambda\, \delta_{i,j}\right]\, \hat{n}_i\, \hat{n}_j \;+\; \lambda\, \hat{N} \tag{A3.2}$$

where $\hat{N}$ is the total density operator. For λ sufficiently large the matrix $v'_{i,j} = v_{i,j} - \lambda\delta_{i,j}$ in the preceding equation (A1.2) is negative definite. Therefore one can apply the transformation (1.5) even in this case. In fact, diagonalizing the symmetric negative-definite matrix (the matrix v can generally be chosen symmetric in a quadratic form like A3.1)

$$v'_{i,j} \;=\; \sum_k U_{k,i}\, \alpha_k^2\, U_{k,j} \tag{A3.3}$$

one can decompose the quadratic form

$$\sum_{i,j} v'_{i,j}\, \hat{n}_i\, \hat{n}_j \;=\; \sum_k \;-\; \alpha_k^2\, \hat{O}_k^2 \tag{A3.4}$$

where

$$\hat{O}_k \;=\; \sum_j U_{k,j}\, \hat{n}_j \tag{A3.5}$$

are single particle commuting operators satisfying

$$\left[\hat{O}_k,\, \hat{O}_j\right] \;=\; 0 \quad and \quad \left[\hat{O}_k,\, \hat{N}\right] \;=\; 0 \quad \forall\, k, j \tag{A3.6}$$

Therefore the calculation of

$$\begin{aligned} e^{-\sum_{i,j} v'_{i,j}\, \hat{n}_i\, \hat{n}_j} \;&=\; \prod_k e^{\alpha_k^2\, \hat{O}_k^2} \qquad using\ (A3.6) \\ &=\; \int \prod_k d\sigma'_k\, e^{-\sum_k \sigma'_k \alpha_k\, \hat{O}_k \,-\, \frac{1}{2}\, \sigma'^2_k} \end{aligned} \tag{A3.7}$$

Finally with the further change of variables:

$$\sigma_k = \sum_j U_{k,j}\, \sigma'_j \tag{A3.8}$$

using eq. (A3.7) and definition (A3.3)

$$e^{\sum_{i,j} v_{i,j}\, \hat{n}_i\, \hat{n}_j} = \int \prod_k d\sigma'_k\, e^{-\sum_{k,j} \sigma'_j\, (\lambda - v)^{1/2}_{k,j}\, \hat{n}_j}\; e^{\sum_k -\frac{1}{2}\sigma'^2_k}\; e^{-\lambda \hat{N}} \tag{A3.9}$$

In practice it is convenient to choose λ equal to the maximum eigenvalue of the matrix v. In this case, in fact we need one less integration variable in the previous transformation.

APPENDIX 4

An efficient way for generating normally distributed variables is to consider a gaussian distribution in two dimensions (x_1, x_2) for which the number of points in a differential area is proportional to:

$$e^{-\frac{1}{2}(x_1^2+x_2^2)}\, dx_1\, dx_2 \tag{A4.1}$$

In terms of the usual polar coordinates

$$r = (x_1^2 + x_2^2)^{\frac{1}{2}}, \qquad \theta = \tan^{-1}\frac{x_2}{x_1} \tag{A4.2}$$

the distribution is

$$e^{-\frac{1}{2}r^2 r}\, dr\, d\theta$$

or, if $u = e^{-\frac{1}{2}r^2}$, $v = \frac{1}{2\pi}\theta$, the distribution is constant for $0 \leq u \leq 1$ and $0 \leq v \leq 1$.

Hence if we generate U and V uniformly between 0 and 1 then the corresponding values of

$$x_1 = \cos(2\pi v)(-2\ln u)^{\frac{1}{2}} \quad x_2 = \sin(2\pi v)(-2\ln u)^{\frac{1}{2}}$$

will be distributed normally. The routine for generating a pseudo-random sequence of numbers between 0 and 1 is standard in any computer and therefore we have all the ingredients for computing the iteration in eqs. (2.18) and (2.21).

////

APPENDIX 5

Consider $N_T = 2^k$ with $k \longrightarrow \infty$. Define

$$S_k = \frac{Z(N_T)}{Z_+(N_T)} \tag{A5.1}$$

From (A5.1) S_k is such that $\forall k,\ 0 \leq S_k < 1$ (from $Z = Z_+ - Z_-$ being Z_+, Z, Z_- positive).

$$a_0 = \frac{1}{2} < \psi_0 | \psi_G > \tag{A5.2}$$

then:

$$\begin{cases} S_k \geq a_0 & \forall\, k \\ S_k \to 0 & \textit{exponentially in } N_T \end{cases} \tag{A5.3}$$

PROOF:

$< \psi_0 | \psi_G >$ can be written as:

$$\begin{aligned} < \psi_0 | \psi_G > &= \lim_{k \to \infty} \frac{< \psi_0 \,|\, e^{-2^k \,\Delta T \,\hat{H}} \,|\, \psi_0 >}{|| \, e^{-2^k \,\Delta T \,\hat{H}} \,|\, \psi_0 > \,||} > 0 \\ &= \lim_{k \to \infty} \frac{< \psi_0 \,|\, e^{-2^k \,\Delta T \,\hat{H}} \,|\, \psi_0 >}{< \psi_0 \,|\, e^{-2^{k+1} \,\Delta T \,\hat{H}} \,|\, \psi_0 >^{\frac{1}{2}}} > 0 \\ &= \lim_{k \to \infty} \frac{Z(2^k)}{Z^{\frac{1}{2}}(2^{k+1})} \end{aligned} \tag{A5.4}$$

The convergence in the previous limit means that for some $k > k_0$, using the definition (A5.1), the following inequality holds:

$$a_0 \leq \frac{Z(2^k)}{Z^{\frac{1}{2}}(2^{k+1})} = \frac{S_k}{S_{k+1}^{\frac{1}{2}}} \frac{Z_+(2^k)}{Z_+^{\frac{1}{2}}(2^{k+1})} \tag{A5.5}$$

Hence from app.1b

$$S_{k+1} \leq \frac{S_k^2}{a_0^2} \tag{A5.6}$$

By iterating the preceding inequality:

$$\frac{S_{k+N}}{a_0^2} \leq \left[\frac{S_k^2}{a_0^2} \right]^{2^N} \tag{A5.7}$$

Therefore if for some $k > k_0$ $S_k < a_0$ then $S_K \to 0$ in an exponential way with respect to N_T. Hence the relation (A5.3) holds.

REFERENCES

1. Anderson P. W., preprint
2. Blankenbecker R., Scalapino D. J. and Sugar R. L., Phys. Rev. D 24 (1981) 2278
3. Car R. and Parrinello M., Phys. Rev. Lett. 55 (1985) 2471
4. Ceperley D. M., "Recent Progress in Many-Body Theories" Springer Verlag, Berlin (1981) 262
5. Ceperley D. M. and Alder B. J., J. Chem. Phys. 81 (1984) 5833
6. Fest M. D., Fleck J. A. and Steiger A., J. Comp. Phys. 47 (1982) 412
7. Gunsteren W. F. and Berendsen H. J., Mol. Phys. 45 (1982) 637
8. Hirsh J. E., Phys. Rev. B 31 (1985) 4403
9. Hirsh J. E. and Scalapino D. J., Phys. Rev. Lett. 56 (1986) 273..
10. Kalos M. H., "Monte Carlo Method in Quantum Physics", NATO ASI Series, D. Reidel Publ. Co.–Dordrecth (1984) 19
11. Koonin S. E., Sugiyama G. and Friedriech H., to be published
12. Kosterlitz J. M., Solid State Phys. 7 (1974) 1046
13. Lieb E. H. and Wu F. Y., Phys. Rev. Lett. 20 (1968) 1445
14. Nobile A. and Roberto V., Comp. Phys. Comm. 42 (1986) 233
15. Ovchinnikov A. A., Sov. Phys. JEPT 30 (1970) 1160
16. Parisi G. and Yougshi W., Scientia Sinica 24 (1981) 483
17. Shiba S. and Pincus P., Phys. Rev. B 5 (1972) 1982
18. Soos Z. G. and Ramasesha S., Phys. Rev. B 29 (1984) 5410
19. Takahashi M., Prog. Theor. Phys. 43 (1970); 42 (1969) 1098
20. Takahashi M., J. Phys. C 10 (1977) 1289
21. White S. R., Wilkins J. and Wilson K., Phys. Rev. Lett. 56 (1986) 4..
22. Yokoyama H. and Shiba H., J. Phys. Soc. of Japan 56 (1987) 1490

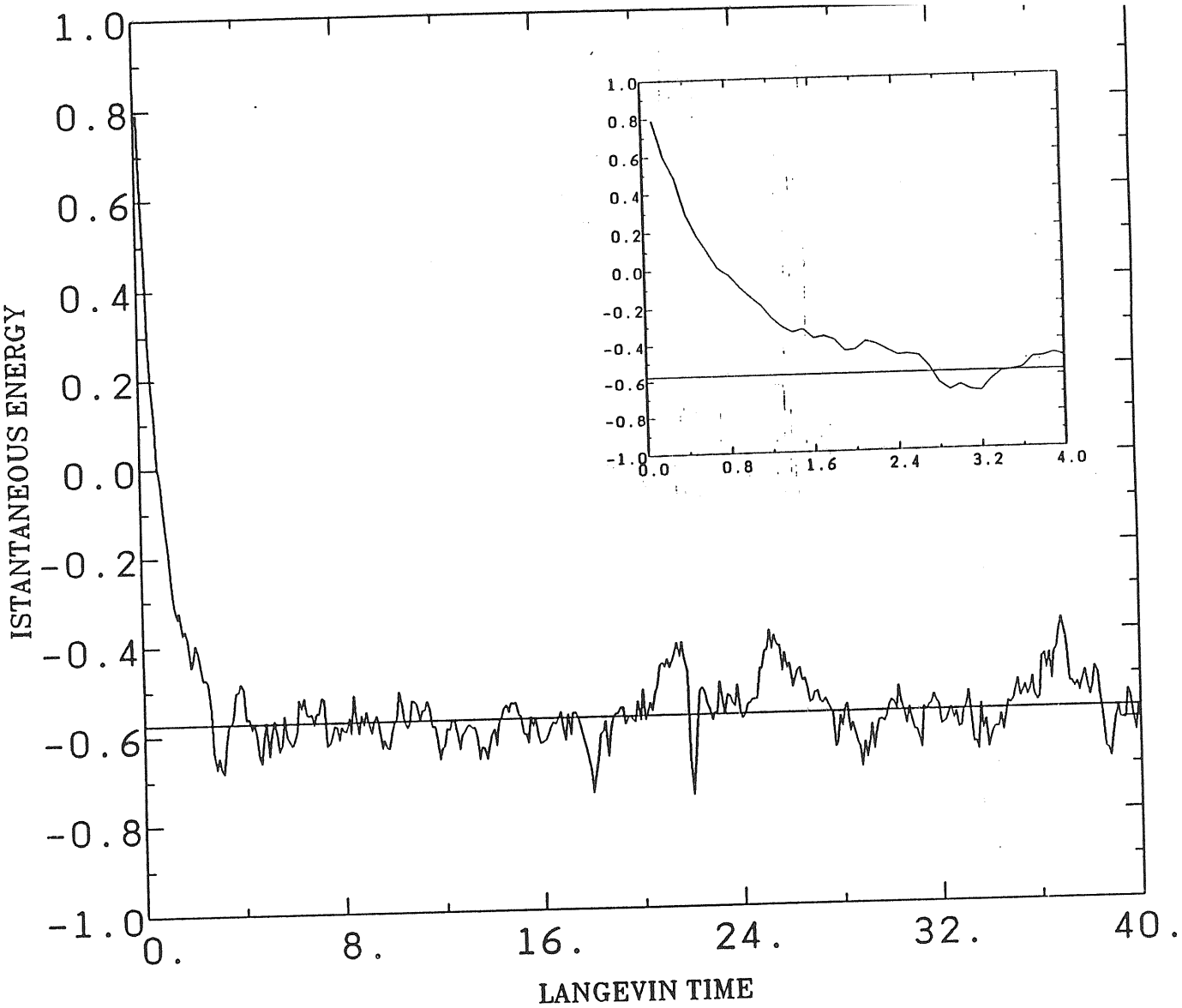

FIG. 1. Typical Langevin evolution (eq. 2.22) of the instantaneous energy (eq. 2.6) with respect to the Langevin time. The horizontal line is drawn at the exact ground state energy. The strength of interaction $U = 4$, the imaginary time (inverse effective temperature) step $\Delta T = 0.05$ the, number of such imaginary time steps $N_T = 320$ and the number of sites $N = 8$ are kept fixed. In all the Figs. the number of particles is chosen according to the half filled conditions.

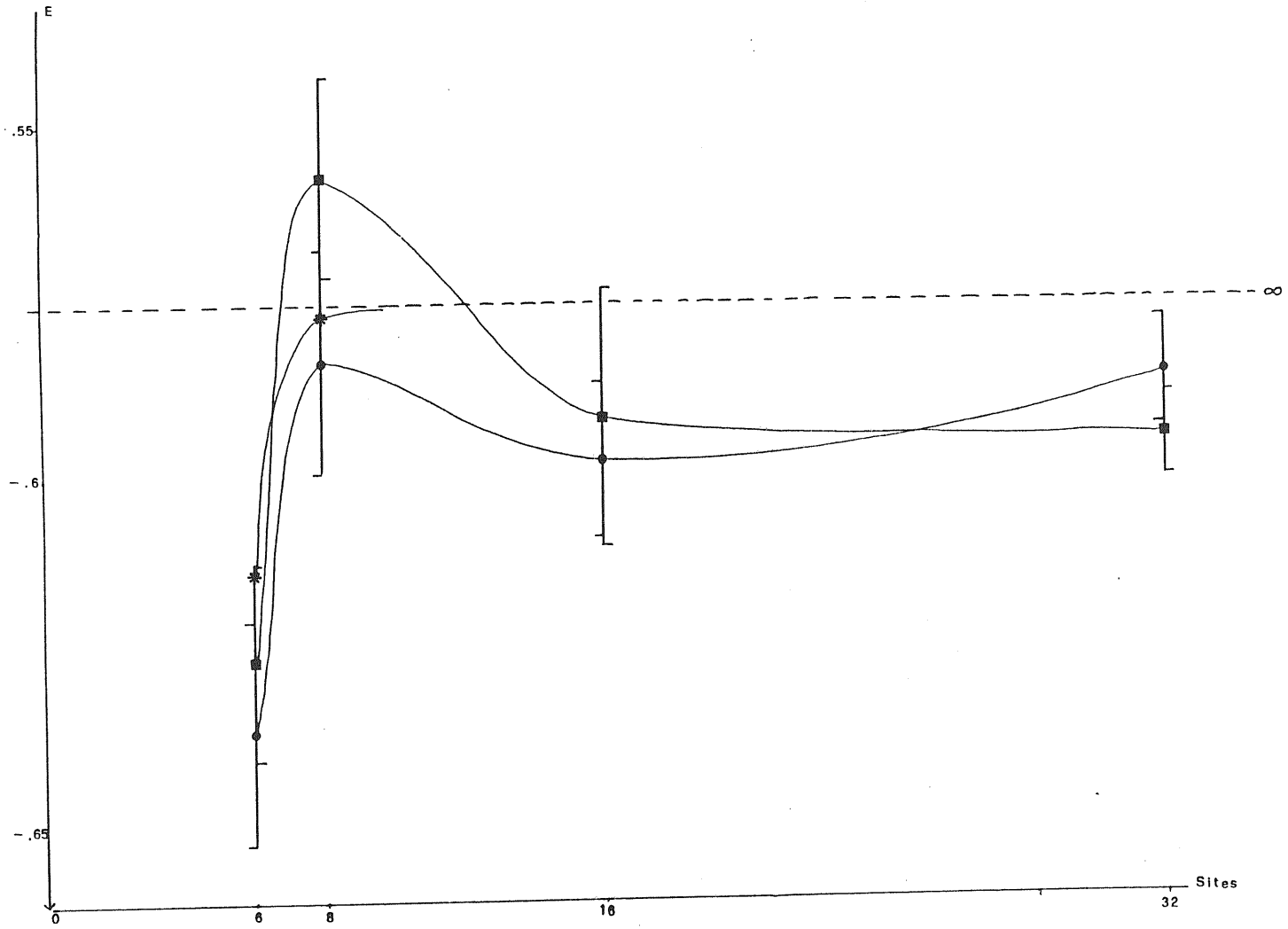

FIG. 2. Average values of the estimated energy (eq. 2.6) as a function of size N using the first order Langevin evolution (eq. 2.19). The asterisk gives the corresponding exact values ($U = 4$, $\Delta T = 0.05$) at the given size and the square and circle dots the estimated energies for different number of imaginary time steps, 128 and 256 respectively.

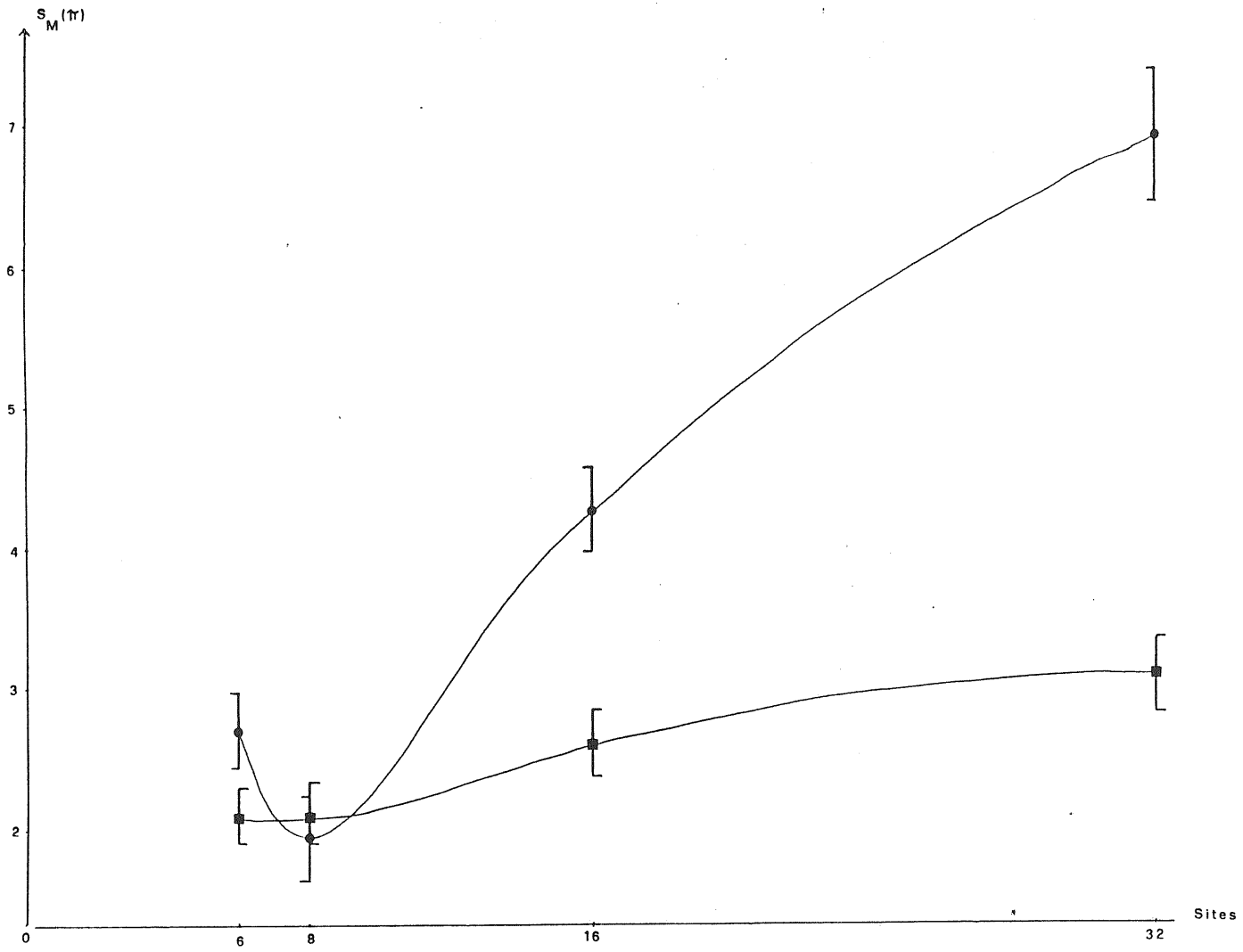

FIG. 3. Size dependence of the magnetic structure factor (eq. 4.48) for $q = \pi$ using the conjugate variables σ (see eq. 4.67). The statistical simulation were done in the same conditions as for the results shown in Fig.2 and we used the same notations.

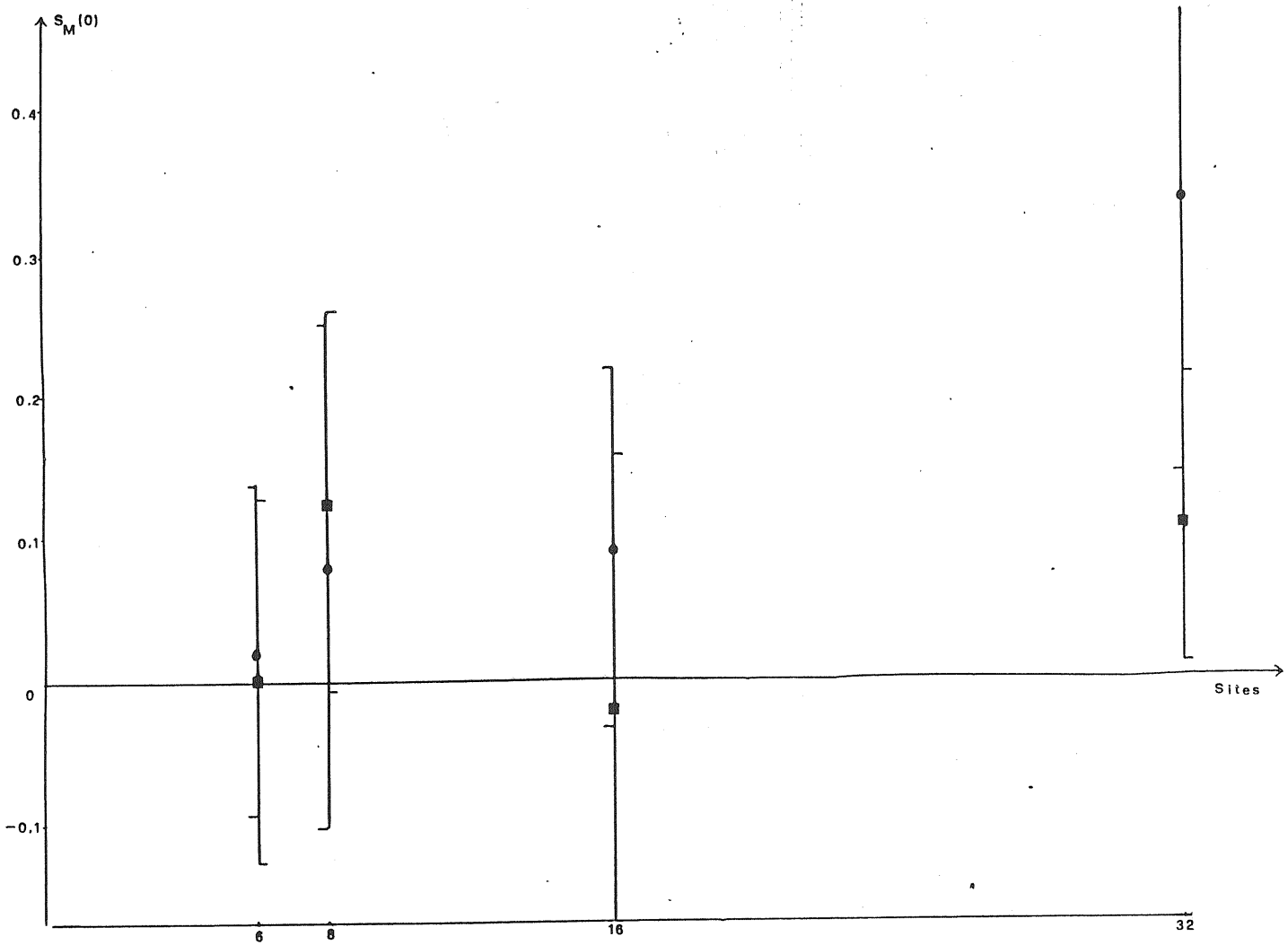

FIG. 4. Size dependence of the magnetic structure factor (eq. 4.49) for $q = 0$ using the conjugate variables σ (see eq. 4.67). The statistical simulation were done in the same conditions as for the results shown in Fig.2 and we used the same notations.

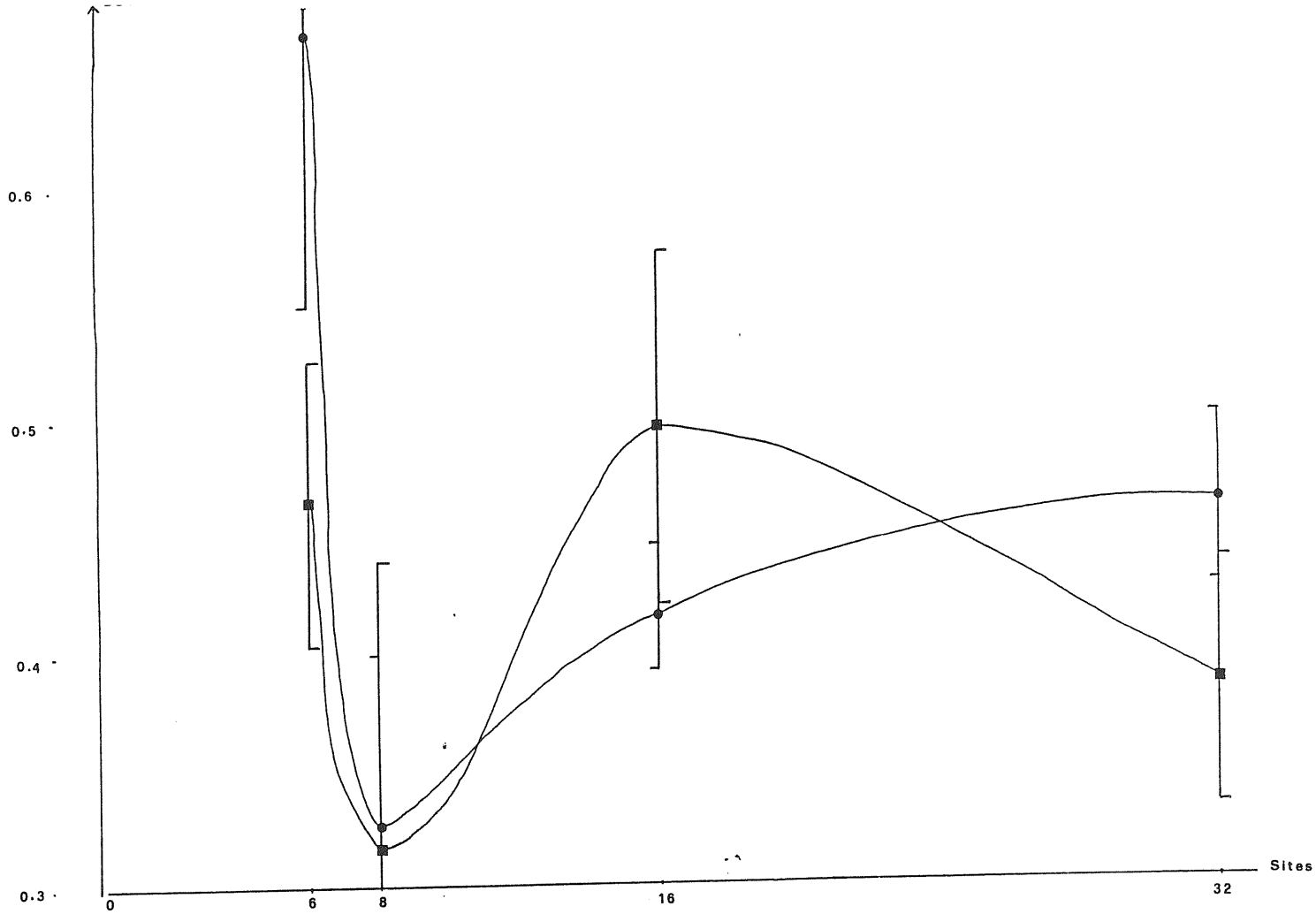

FIG. 5. Size dependence of the estimated Cooper–correlation functions at $q = 0$ and for next neighbour lattice sites ($\tau = +1$ in 4.50). The statistical error is large because in this case only one sample for each Langevin step is updated; several samples in fact can be obtained at different imaginary times reducing the statistical errors (see Fig.16). The statistical simulation were done in the same conditions as for the results shown in Fig.2 and we used the same notations.

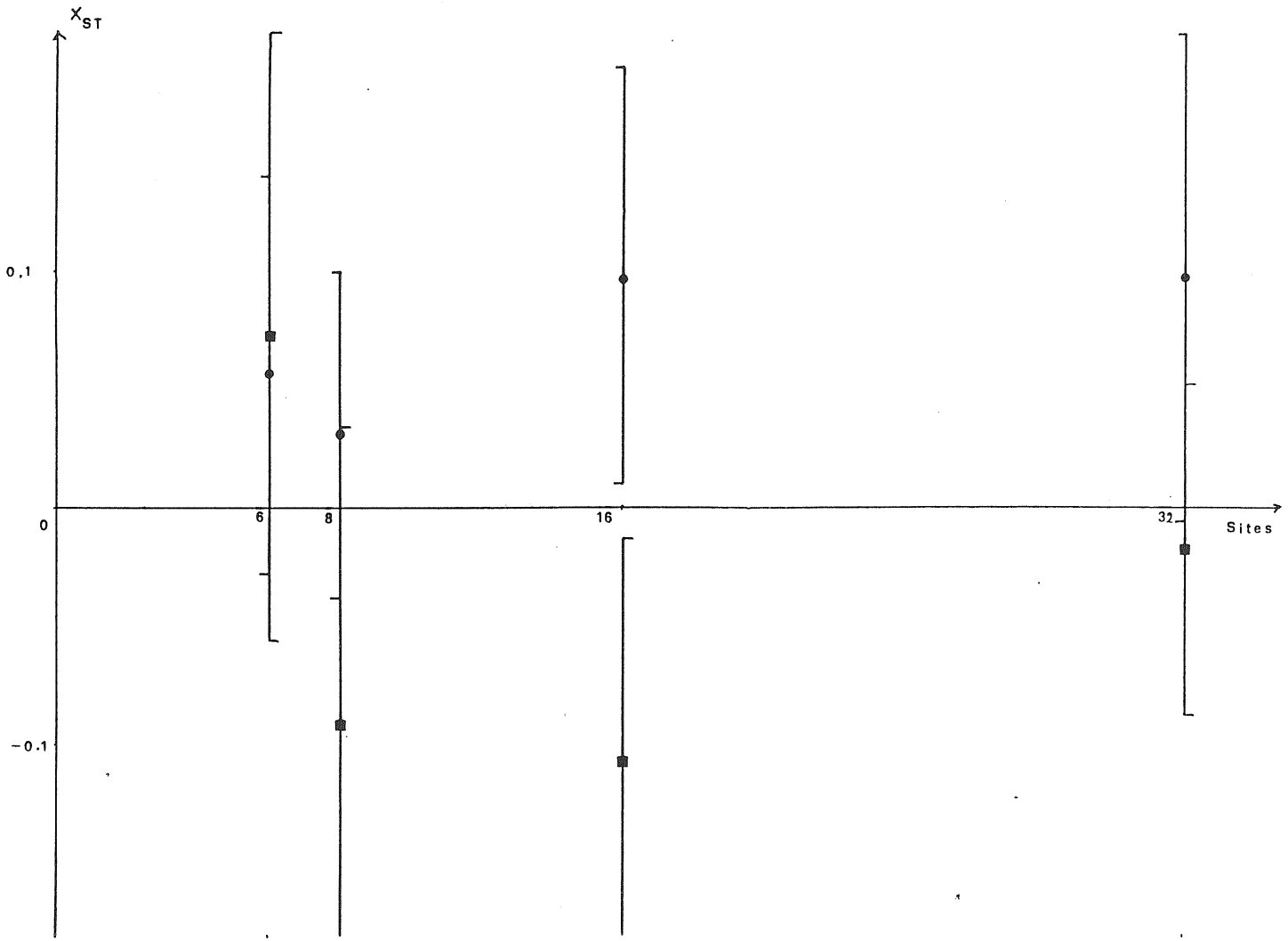

FIG. 6. Size dependence of the estimated spin susceptibility using the conjugate variables σ. The exact value of χ_{st} for such finite system without magnetization vanishes.

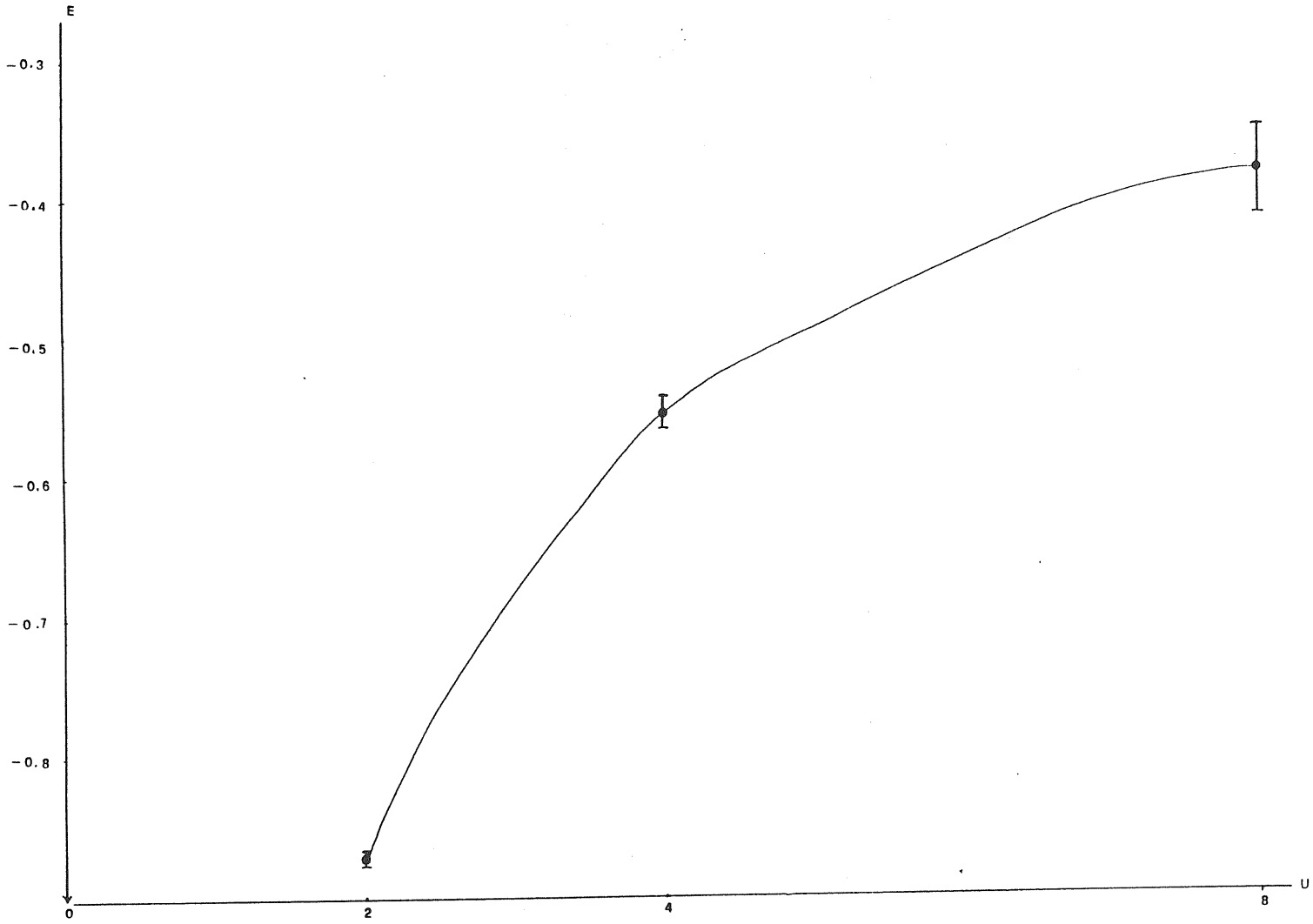

FIG. 7. Estimated values of the ground state energy for different values of the interaction ($N = 8$, $U\Delta T = \frac{1}{5}$ and $N_T = 256$).

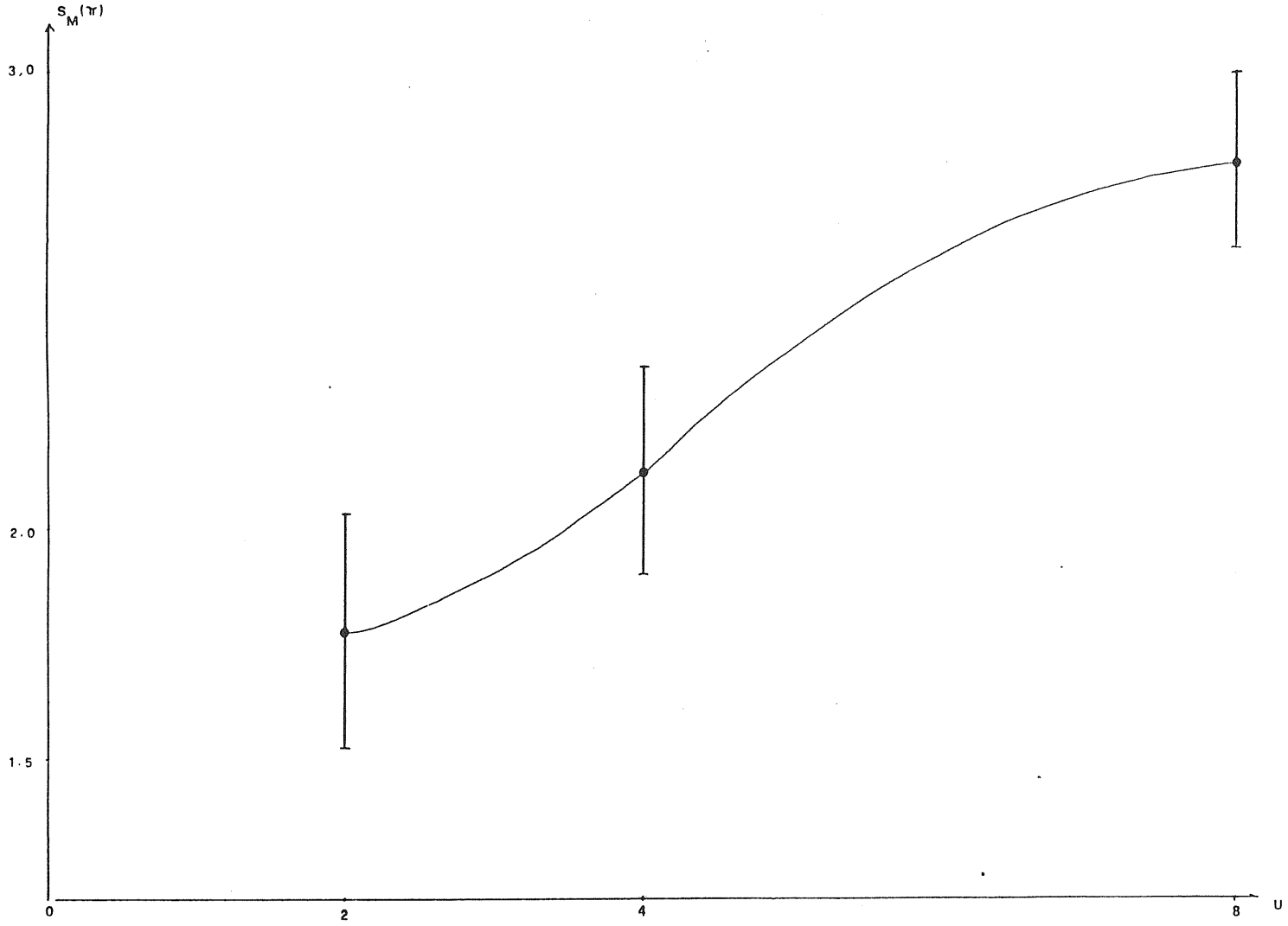

FIG. 8. Estimated values for the magnetic structure factor ($q = \pi$) for different values of the interaction U using the conjugate variables σ ($N = 8$, $U\Delta T = \frac{1}{5}$ and $N_T = 256$).

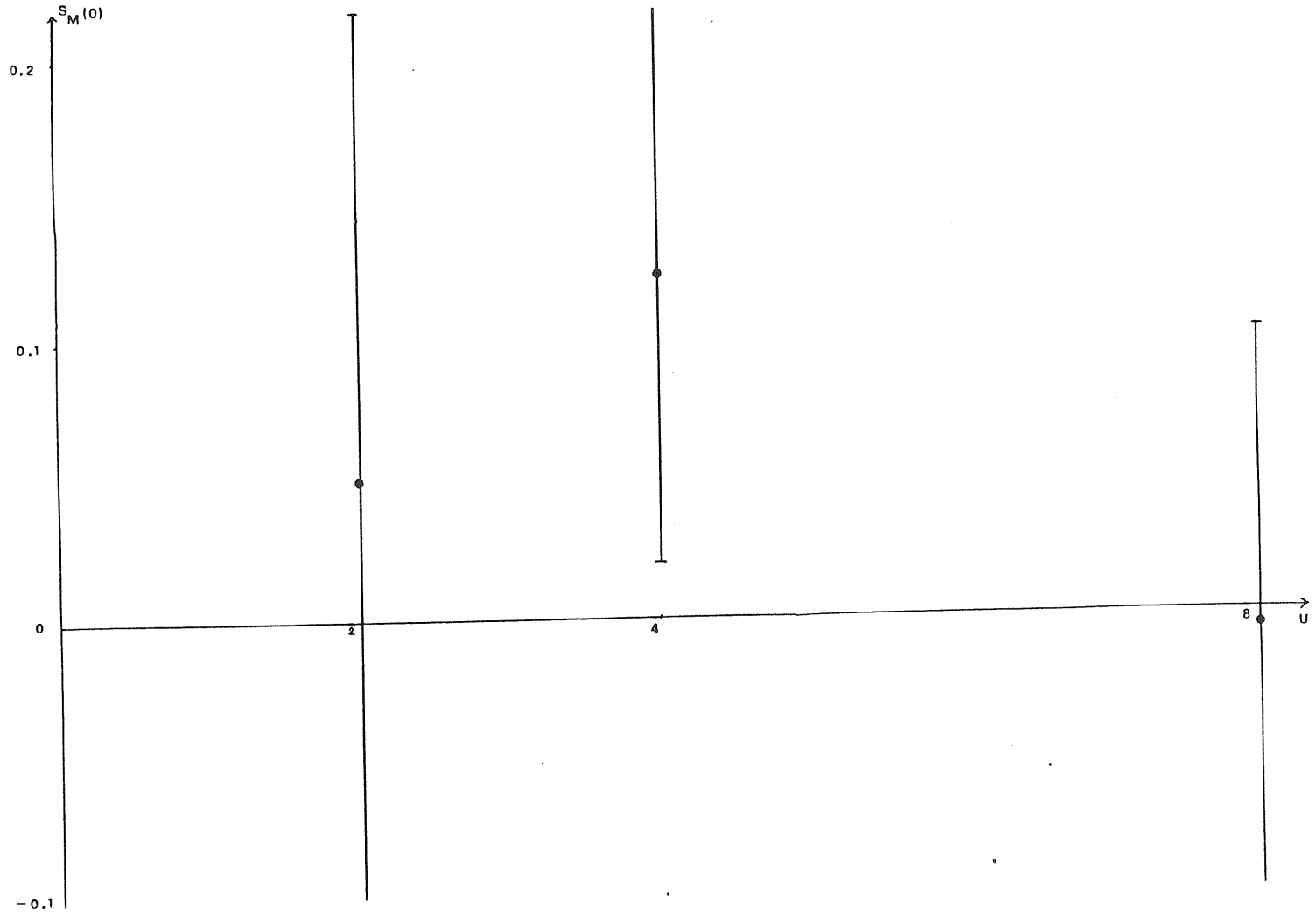

FIG. 9. Estimated values for the magnetic structure factor ($q = 0$) for different values of the interaction U using the conjugate variables σ ($N = 8$, $U\Delta T = \frac{1}{5}$ and $N_T = 256$).

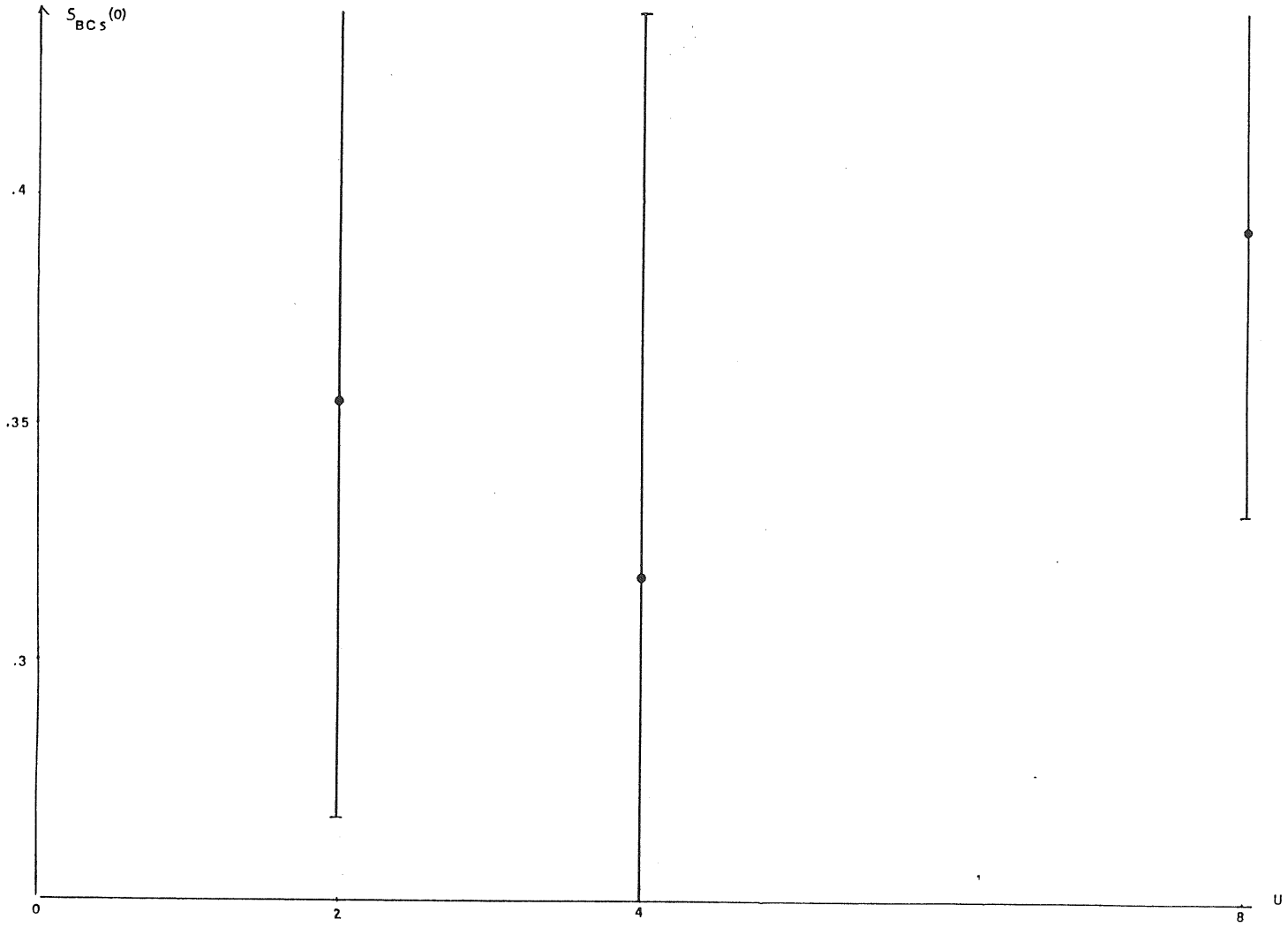

FIG. 10. Estimated (as in Fig.5) values of the Cooper correlation function for different values of the interaction ($N = 8$, $U\Delta T = \frac{1}{5}$ and $N_T = 256$).

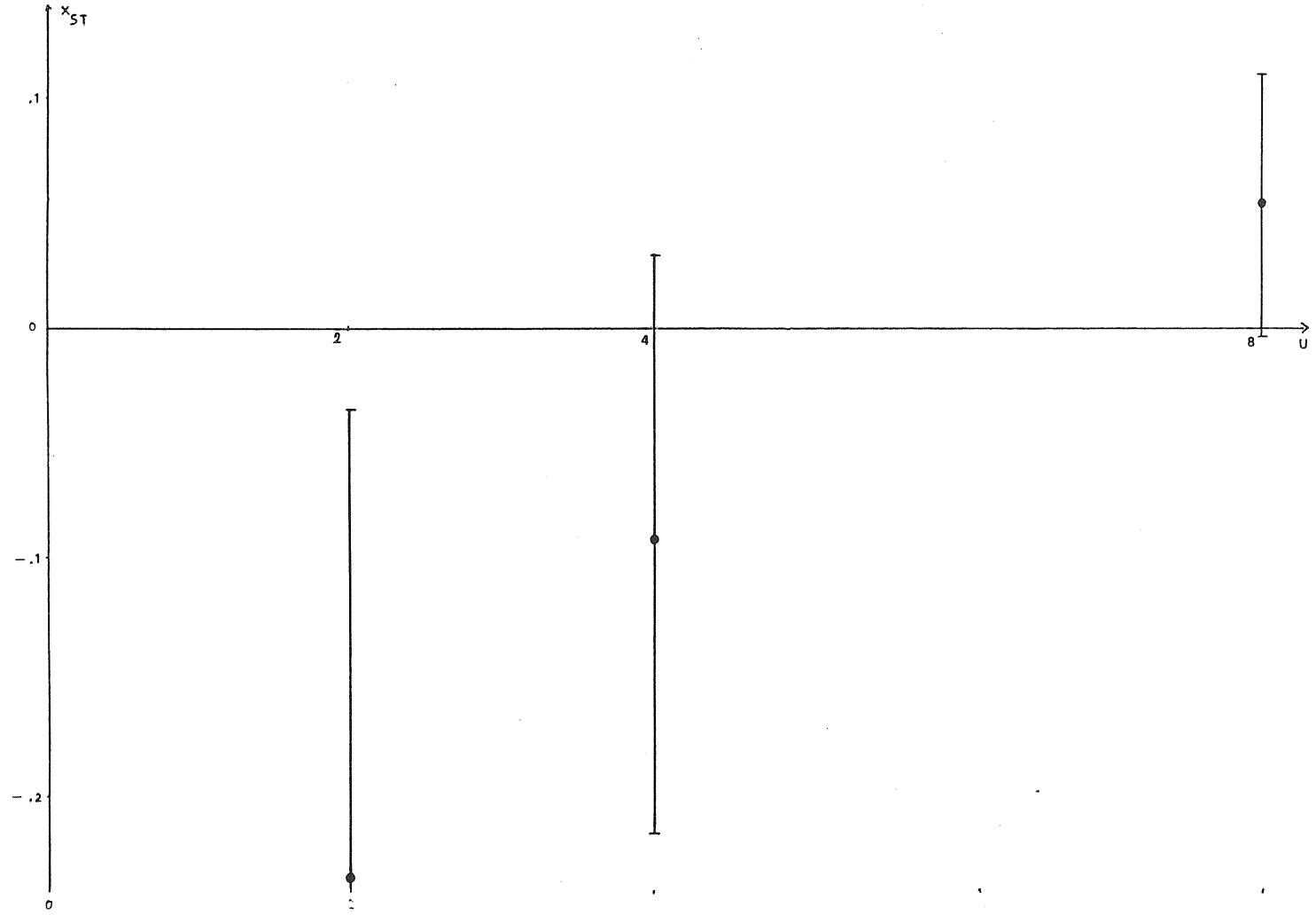

FIG. 11. Estimated spin susceptibility (the exact value vanishes) using the conjugate variables as a function of the interaction ($N = 8$, $U\Delta T = \frac{1}{5}$ and $N_T = 256$).

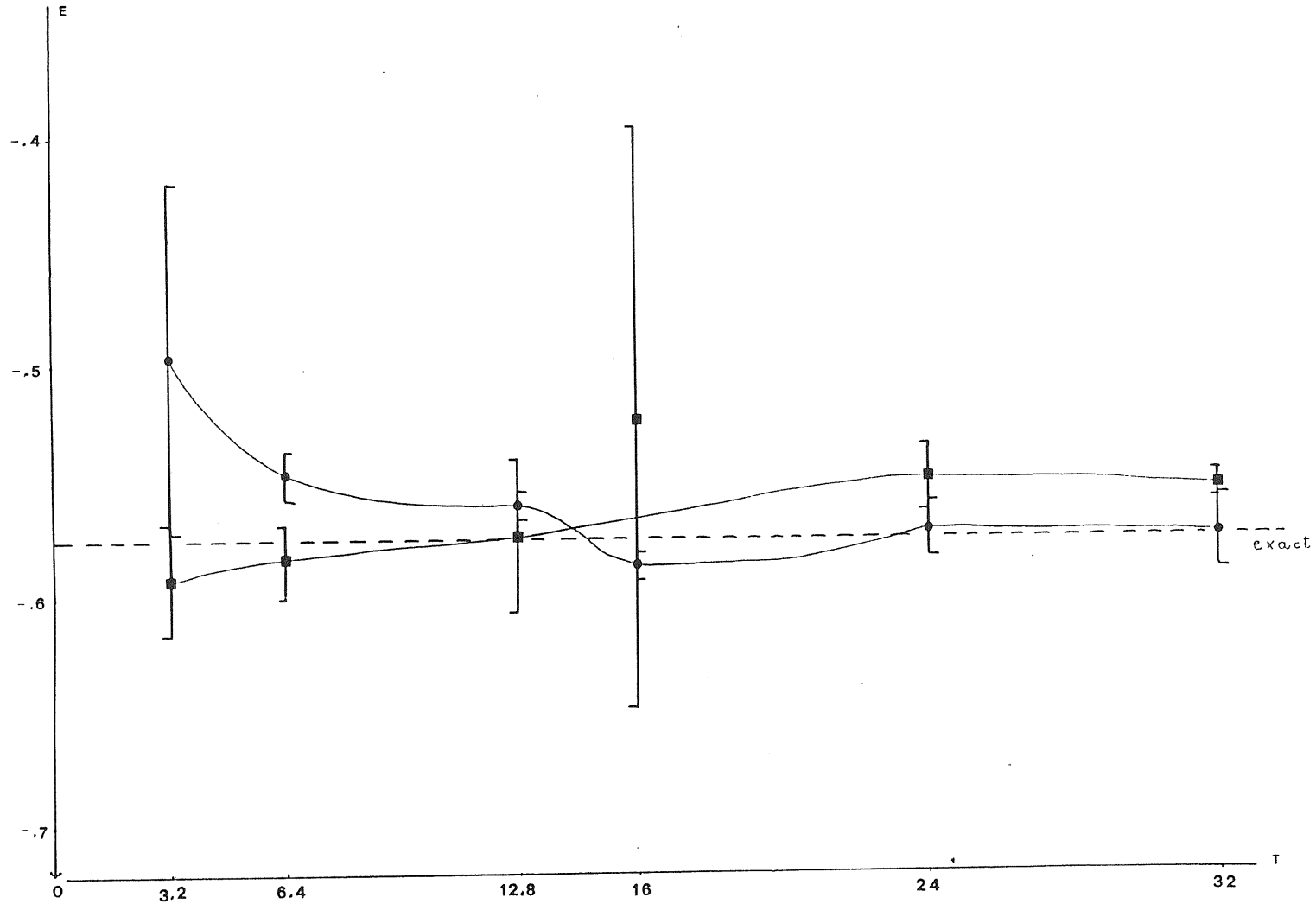

FIG. 12. Convergence in imaginary time T for estimated energies (eq. 4.62) sampled in the positive (circle dot) or in the negative (square dot) determinant sign. $N = 8$, $U = 4$ and ΔT are fixed in the simulation.

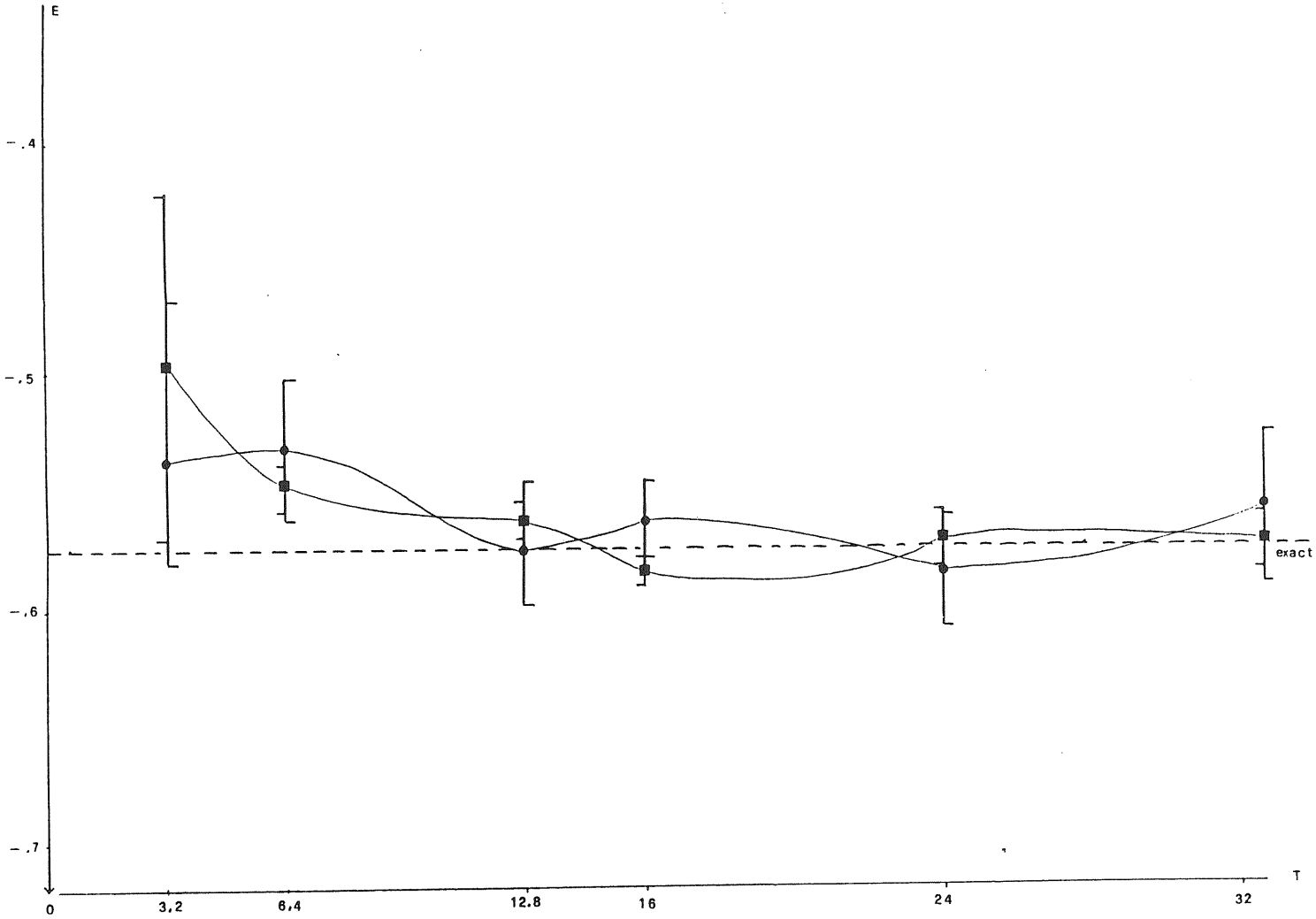

FIG. 13. Convergence in imaginary time for estimated energies with two different methods. The dot and the square points correspond to the methods derived in eq. (2.6) and eq. (4.62). $N = 8$, $U = 4$ and ΔT are fixed in the simulation.

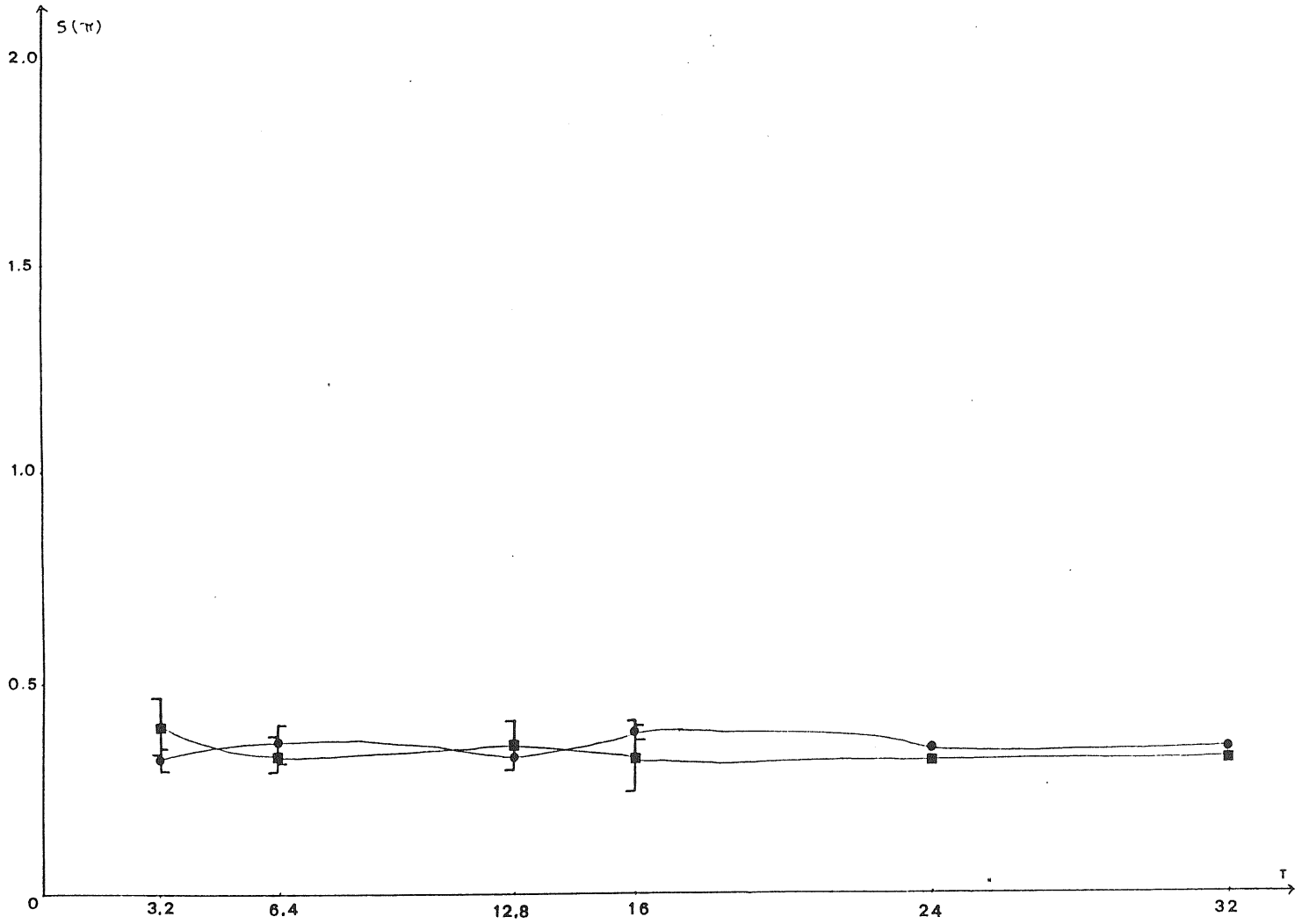

FIG. 14. Imaginary time convergence of the estimated density correlation functions for $q = \pi$ (eq. 4.49 and eq. 4.61). The estimated values were sampled in the positive (dots) or negative (square dots) determinant region ($N = 8$, $U = 4$ and ΔT).

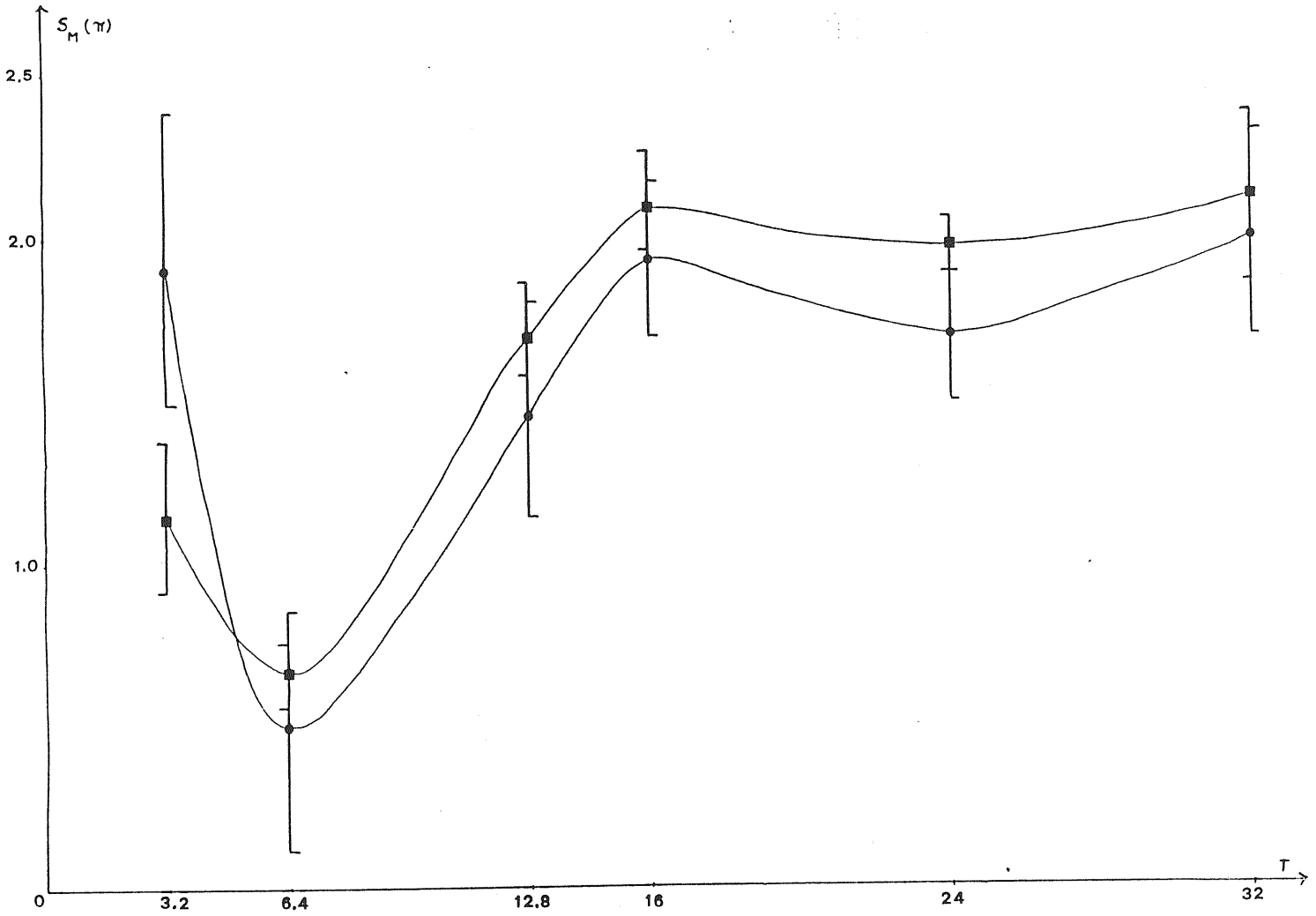

FIG. 15. Imaginary time convergence of the estimated magnetic correlation functions for $q = \pi$ (eq. 4.48). The estimated values were calculated using either the conjugate variables σ (see eq. 4.67) or by the direct evaluation of the Green's function (eq. 4.61) ($N = 8$, $U = 4$ and ΔT).

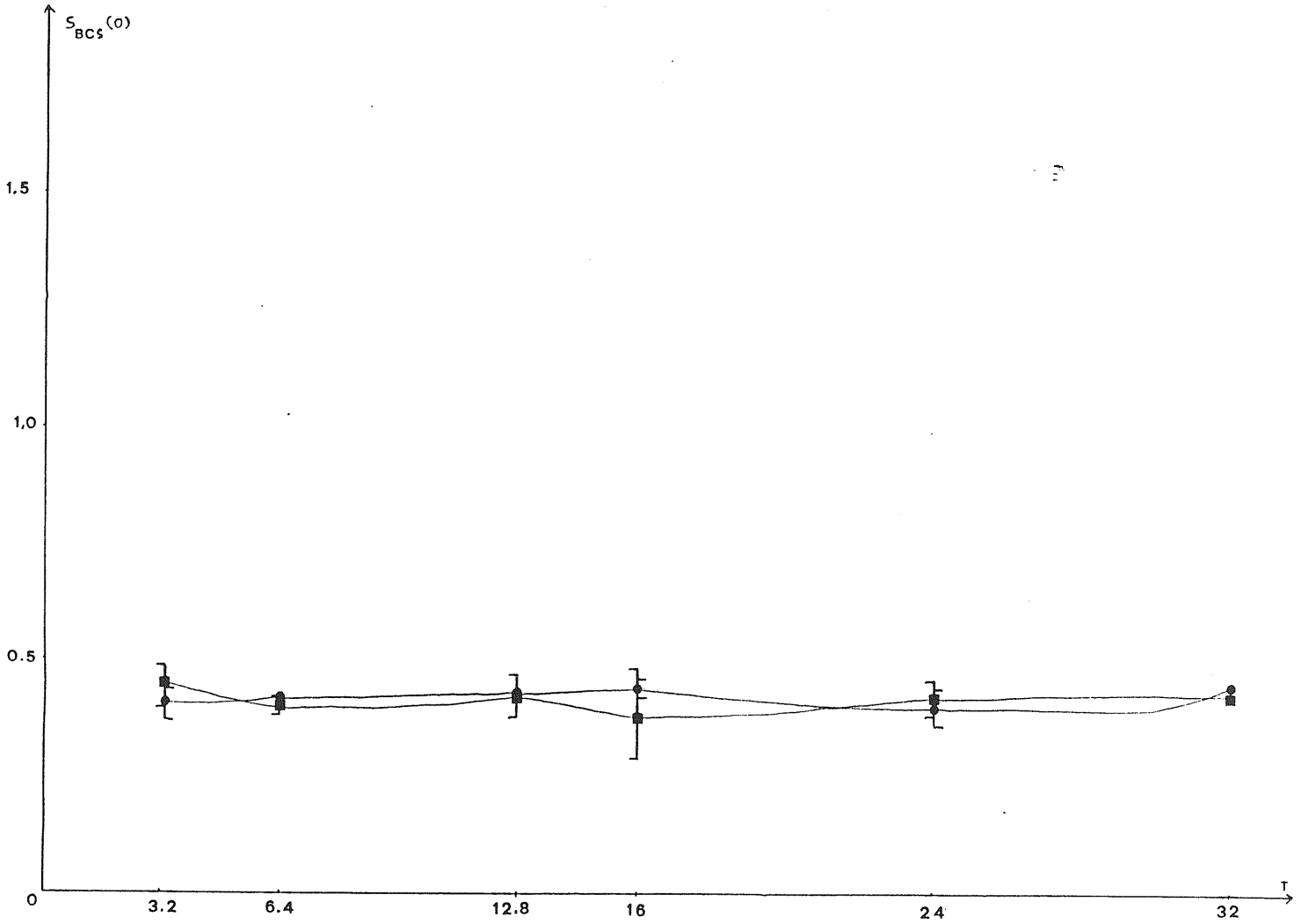

FIG. 16. Imaginary time convergence of the estimated Cooper–correlation functions at $q = 0$ and for next neighbour lattice sites ($\tau = +1$ in 4.50) Cooper correlation functions in the positive (dots) or negative (square dots) determinant regions ($N = 8$, $U = 4$ and ΔT).