Quantum Monte Carlo method in details.

I. CONTINUOUS AND DISCRETE HUBBARD-STRATONOVICH TRANSFORMATIONS

The HS transformation is based on identity :

$$\exp\{\frac{1}{2}A^2\} = (2\pi)^{-1/2}\int\limits_{-\infty}^{+\infty} dx \exp\{-\frac{1}{2}x^2 - xA\} \tag{1}$$

This identity allows to map interacting fermion system onto the system of noninteracting fermions coupled with fluctuating auxilary field. One uses a path integral formulation of a problem to eliminate the interaction term. We divide the imaginary time interbal $[0,\beta]$ into Lequal subintervals of width $\Delta\tau : L\Delta\tau = \beta$.

After doing that we can rewrite equation for the partitionfunction Z as:

$$Z = Tre^{-\beta(H_0+H_1)} = Tr\prod_{i=1}^{L} e^{-\Delta\tau(H_0+H_1)} \approx Tr\left[T_\tau \exp\left[-\int\limits_0^\beta d\tau(H_0+H_1)\right]\right] + O((\Delta\tau)^2) \tag{2}$$

Now we can describe notion *continuous* and *descrete* HB.

A. Continuous

Let us consider the hamiltonian with interaction term in the following form:

$$\mathcal{H}^i = U\sum_i [n_i n_{i+1} - \frac{1}{2}(n_i + n_{i+1})], \tag{3}$$

then using well-known relation for the occupation numbers:

$$n_i n_{i+1} = -\frac{1}{2}(n_i - n_{i+1})^2 + \frac{1}{2}(n_i + n_{i+1}) \tag{4}$$

we can rewrite the interaction part of the hamiltonian as

$$\mathcal{H}^i = U\sum_i [n_i n_{i+1} - \frac{1}{2}(n_i + n_{i+1})] = -\frac{U}{2}\sum_i (n_i + n_{i+1})^2. \tag{5}$$

Now using the HS trasformation we get for each time interval:

$$\exp\left[\int_0^\beta d\tau \frac{U}{2}\sum_i (n_i+n_{i+1})^2 = (2\pi)^{-N/2}\int\prod_{i=1}^{N} dx_{i,i+1}\exp\int_0^\beta d\tau\left[-\frac{1}{2}x_{i,i+1}^2 - x_{i,i+1}\sqrt{U}(n_i+n_{i+1})\right]\right],$$

where $x_{i,i+1}$ is a bosonic field associated with the link $i \to i+1$.

Now the Hamiltonian is has quadratic form in fermion operators, the trace over the fermionic degree of freedom can be taken analytically, and the partition function takes the form:

$$Z = (2\pi)^{-N/2}\int\prod_{i=1}^{N} dx_{i,i+1} e^{-S_b}\det\left[1 + T_\tau\left[\int_0^\beta d\tau h(\tau)\right]\right],$$

where $S_b = \int_0^\beta d\tau \sum_i \frac{1}{2}x_{i,i+1}^2$,is the bosonic part of the action.

$h(\tau)$ is the $N \times N$ matrix, where N is the size of the system.
Let us define $N \times N$ matrix for each time slice:

$$B_l = \exp(-\Delta\tau h(\tau_l)).$$

Using this definition we can write

$$Z = (2\pi)^{-NL/2} \int \prod_{i=1}^{N} dx_i e^{-S_b} \det\left[1 + B_L B_{L-1} ... B_1\right].$$

B. Descrete

Main Idea: fermion occupancies can take only the values 0 and 1 and the files that can take only two values must be enough to eliminate the fermion interaction.

We use the following identity:

$$e^{-\Delta\tau U n_\uparrow n_\downarrow + (\Delta\tau U/2)(n_\uparrow + n_\downarrow)} = \frac{1}{2} \sum_{s=\pm 1} e^{\lambda s (n_\uparrow - n_\downarrow)}, \tag{6}$$

where $\lambda = \operatorname{arccosh}(e^{\Delta\tau U/2})$ and the discrete field s is an Ising-like variable taking the values ± 1.
Taking the trace over fermion degree of freedom we get:

$$Z = \sum_{s=\pm 1} \det\left[1 + T_\tau\left[-\Delta\tau \sum_l h(l)\right]\right],$$

where $h(l)$ is the same $N \times N$ matrix, but with descrete variables s instead continuous x.
Using the same expression for B_l we get the following fomr for the partition function:

$$Z = \sum_{s_l=\pm 1} \det\left[1 + B_L B_{L-1} ... B_1\right].$$

(Notice: **There is NO bosonic part!**)

C. A few words about Metropolis algorithm.

Now we need to go over all spin configurations and compute the corresponding action. While walking we accept or reject new configuration in a way that assures that once the equiliblium has been reached the probability of a particular field configuration is proportiaonal to $\exp(-S)$, where S is the action. For the fermionic system the effective action $\exp(-S) = \exp(-S_b)\det(M)$ is non-local and is compuatation is very time consuming.

II. METHODS OF SOLUTION

As explained in the previous sections, lattice models of correlated fermions can be mapped, in the limit of infinite coordination number, onto a single-impurity model which has to satisfy a self-consistency condition. This condition specifies, for a given lattice, the relation between the Weiss function $\mathcal{G}_0$ (entering the impurity model effective action) and the local Green's function G. On the other hand, G itself is obtained by solving the effective impurity model. Hence, we have a coupled problem to solve for both G and $\mathcal{G}_0$. In practice, all methods deal with this coupled problem in an *iterative* manner: the local Green's function is obtained by solving the impurity effective action given a $\mathcal{G}_0$ (in the first step a guess for $\mathcal{G}_0$ is used). Then, the calculated G (and the self-energy Σ) is used as an input into the self-consistency condition to produce a new Weiss function $\mathcal{G}_0$. The process is iterated until a converged solution $(G, \mathcal{G}_0)$ is reached. Knowing this converged solution, all $\boldsymbol{k}$-dependent response functions can be constructed from the impurity model response functions.

To be definite, we concentrate in this section on the case in which the impurity model effective action has the form given by:

$$S_{eff} = -\int_0^\beta d\tau \int_0^\beta d\tau' \sum_\sigma c_\sigma^+(\tau)\mathcal{G}_0^{-1}(\tau-\tau')c_\sigma(\tau') + U\int_0^\beta d\tau\, n_\uparrow(\tau)n_\downarrow(\tau) \tag{7}$$

that corresponds to the local site of the single-impurity Anderson model. In the LISA framework, the $\{c,\ c^+\}$ operators are associated with a local fermionic variable of the lattice problem.

The most difficult step in the iterative procedure is the repeated solution of the impurity model, for an essentially arbitrary $\mathcal{G}_0$ (*i.e.* an arbitrary conduction electron effective bath). Even though spatial degrees of freedom have been eliminated, the impurity model remains a true many-body problem. It is crucial to use *reliable* methods to handle it. Fortunately, quantum impurity models have been studied for over thirty years, and several techniques are available. In this section we review some of these techniques along with some recently developed ones. In particular, we describe in detail a general numerical method which is based on the exacts diagonalization of small clusters. We then describe a projective technique, inspired by the renormalization group method for impurity models, which can be applied to problems with a separation of energy scales.

In contrast to the solution of the single-impurity problem, the implementation of the self-consistency condition in the numerical methods is relatively straightforward. Even though no rigorous proof exists concerning the convergence of the iterative process, practice has shown that it is usually not difficult to reach a self-consistent solution of the LISA equations. Convergence is usually attained after a few iterations. Close to transition points one encounters critical slowing down of the convergence (in the broken symmetry phase) which can however be easily overcome by standard accelerated convergence methods.

III. QUANTUM MONTE CARLO METHOD

A. A scematic derivation

The most successful method for solving a general impurity problem is due to Hirsch and Fye (1986). Before embarking on a rigorous and self-contained derivation of their method, we describe in this section the algorithm taking a rather different, though less rigorous, approach for the sake of an intuitive understanding of the key ingredients of this method. The method is concerned with the calculation of the local Green's function at finite temperature

$$G(\tau - \tau') \equiv - < Tc(\tau)c^{\dagger}(\tau') >_{S_eff} . \tag{8}$$

- The basic principle of the method can be understood as a discretization of the impurity model effective action Eq. (7)

$$S_{eff} \rightarrow \sum_{\tau\tau'\sigma} c^{+}_{\sigma}(\tau)\mathcal{G}_0^{-1}(\tau,\tau')c_{\sigma}(\tau') + U\sum_{\tau} n_{\uparrow}(\tau)n_{\downarrow}(\tau) \tag{9}$$

  where the imaginary time is discretized in L "slices" $\tau = 1,\ 2,\ ...,\ L$ of size $\Delta\tau$, and the timestep $\Delta\tau$ is defined by $\beta = L\Delta\tau$.

- The remaining quartic term can be decoupled using a discrete Hubbard-Stratonovich transformation (Hirsch, 1983):

$$e^{-\Delta\tau U n_{\uparrow}n_{\downarrow} + (\Delta\tau U/2)(n_{\uparrow}+n_{\downarrow})} = \frac{1}{2}\sum_{s=\pm 1} e^{\lambda s(n_{\uparrow}-n_{\downarrow})} \tag{10}$$

  where $\lambda = \mathrm{arccosh}(e^{\Delta\tau U/2})$ and the discrete field s is an Ising-like variable taking the values ± 1. Performing this transformation at every time-slice, we are led to a quadratic action, and the partition function becomes

$$Z = \sum_{s_\tau=\pm 1}\int D[c,c^{+}]e^{-\sum_{\tau\tau'} c^{+}_{\sigma}(\tau)\mathcal{G}_0^{-1}(\tau,\tau')c_{\sigma}(\tau') + \lambda\sum_{\tau} s_\tau(n_{\uparrow}(\tau)-n_{\downarrow}(\tau))} \tag{11}$$

  with

$$G^{-1}_{\sigma}(\tau,\tau') \equiv \mathcal{G}^{-1}_{0\sigma}(\tau,\tau') + \sigma\lambda s_\tau\delta_{\tau,\tau'+1} \tag{12}$$

  the inverse propagator for a particular realization of the Ising spins $(s_1, ..., s_L)$. The antiperiodic delta function is defined by $\delta_{l,l'+1} = 1$ if $l = l'+1, l = 2, \ldots L-1$,$\delta_{l,l'+1} = -1$ if $l = 1, l' = L$ and is zero otherwise. Its origin is in the proper time ordering of the creation and destruction operators (Blankenbecler, Scalapino and Sugar, 1981). In the actual implementation of the algorithm, Eq. (12) is replaced by

$$G^{-1}_{\sigma,(s_1,\ldots,s_L)}(\tau,\tau') \equiv \mathcal{G}^{-1}_{0\sigma}(\tau,\tau')e^{V} + e^{V} - 1 \tag{13}$$

  where e^V is the diagonal matrix with elements $e^V(\tau,\tau) = e^{\sigma\lambda s_\tau}$. This choice of discretization results from the rigorous derivation following the original Hamiltonian formulation of Hirsch and Fye (1986).

- The replacement of a quartic term for an extra summation on the auxiliary Ising variables $(s_1, \ldots s_L)$ renders the action quadratic and allows us to apply Wick's theorem at each time slice. We can now perform the Gaussian integration of the Grassmann variables, to obtain

$$Z = \sum_{\{s_1,\ldots,s_L\}} \det[G_\uparrow^{-1}(s_1,\ldots,s_L)] \det[G_\downarrow^{-1}(s_1,\ldots,s_L)] \tag{14}$$

  In principle, the trace over the auxiliary field gives the full interacting Green's function

$$G_\sigma = \frac{1}{Z} \sum_{\{s_1,\ldots,s_L\}} \det[G_\uparrow^{-1}(s_1,\ldots,s_L)] \det[G_\downarrow^{-1}(s_1,\ldots,s_L)] G_\sigma(s_1,\ldots,s_L) \tag{15}$$

  this requires the sum over 2^L configurations. Each term in the sum (15) involves the inversion of an LxL matrix as is clear from Eq. (13). In practice, the full trace can only be performed for small values of L.

- Usually, the interacting Green's function is therefore calculated by stochastic Monte Carlo sampling: the term $\det[G_\uparrow^{-1}(s_1,\ldots,s_L)] \det[G_\downarrow^{-1}(s_1,\ldots,s_L)]$ in Eq. (15) is interpreted as a stochastic weight, and configurations $(s_1,\ldots,s_L)$ are generated by a Markov process with a probability corresponding to their statistical weight.

- The Markov process visits configurations of Ising variables $(s_1,\ldots,s_L)$ with a single spin-flip dynamic, in which a possible movement consists in $(s_1, s_2, \ldots, s_k, \ldots, s_L) \rightarrow (s_1, s_2, \ldots, -s_k, \ldots, s_L)$. The formulas given in Sec. III B will allow a rapid calculation of the change in statistical weight, and of the new Green's function for a single spin-flip change.

B. A Rigorous derivation

The above derivation leaves us with the impression that there are two discretizations involved: the one of the bath Green's function, and the subsequent discretization of the functional integral. Using a Hamiltonian description of the general Anderson impurity model one can show (Hirsch and Fye 1986) that only a single well-defined discretization of the partition function need be performed (given by the Trotter break-up). Green's functions corresponding to this discretized partition function can be defined naturally (with the help of the transfer operators). Then, the decoupling using the binary Ising field is performed. Eq. (13) then appears as an (exact) Dyson equation relating different discretized Green's functions.

This section is intended mainly for the reader interested in a detailed understanding of the algorithm (this reader should also realize that, in accordance with the *entire* QMC literature, we define in this section temporal Green's functions *without* the minus-sign in Eq. (8)).

We temporarily introduce the Hamiltonian description of the local impurity problem, which permits a local-in-time description of the partition function. In order to preserve the standard notations for this model, the impurity orbital (that is associated with a local degree of freedom of the original lattice) will be taken as a "d"-orbital in this section. The conduction bath orbitals are numbered from $p = 2, ..., n_s$, and the impurity orbital is equivalently denoted by $a_{1\sigma} \equiv d_\sigma$, *i. e.* corresponds to $p = 1$. The Hamiltonian of a general Anderson impurity model reads

$$\mathcal{H} = \sum_{p\sigma} \widetilde{\epsilon}_p a_{p\sigma}^+ a_{p\sigma} + \sum_{p,\sigma} V_p (a_{p\sigma}^+ d_\sigma + d_\sigma^+ a_{p\sigma}) + \epsilon_d \sum_\sigma d_\sigma^+ d_\sigma + U n_{d\uparrow} n_{d\downarrow} \tag{16}$$

It is written as a sum of terms $\mathcal{H} = \mathcal{H}^0 + \mathcal{H}^i$, where $\mathcal{H}^0$ is quadratic in the fermion operators:

$$\mathcal{H}^0 \equiv \sum_{p\sigma} \widetilde{\epsilon}_p a_{p\sigma}^+ a_{p\sigma} + \sum_{p,\sigma} V_p (a_{p\sigma}^+ d_\sigma + d_\sigma^+ a_{p\sigma}) + (\epsilon_d - U/2) \sum_\sigma n_{d\sigma} \tag{17}$$

whereas $\mathcal{H}^i$ is the interaction term:

$$\mathcal{H}^i = U[n_{d\uparrow}n_{d\downarrow} - \frac{1}{2}(n_{d\uparrow} + n_{d\downarrow})] \tag{18}$$

As in Sec. III A, the imaginary time interval $[0, \beta]$ is now discretized into L time slices, but on the level of the original Hamiltonian $\mathcal{H}$. With $\tau_l = l\Delta\tau$, with $l = 1, ..., L$ and $\Delta\tau \equiv \beta/L$, the partition function is written as

$$Z = \mathrm{Tr}e^{-\beta\mathcal{H}} = \mathrm{Tr}\prod_{l=1}^{L} e^{-\Delta\tau[\mathcal{H}^0+\mathcal{H}^i]} \tag{19}$$

Using the Trotter break-up: $\exp(-\Delta\tau(\mathcal{H}_0 + \mathcal{H}_1)) \sim \exp(-\Delta\tau\mathcal{H}_0)\exp(-\Delta\tau\mathcal{H}_1)$, Z can be approximated by the discretized partition function:

$$Z \simeq Z^{\Delta\tau} \equiv \mathrm{Tr}\prod_{l=1}^{L} e^{-\Delta\tau\mathcal{H}^0}e^{-\Delta\tau\mathcal{H}^i} = \mathrm{Tr}\prod_{l=1}^{L} e^{-\Delta\tau\mathcal{H}^0}\exp[-\Delta\tau[U[n_{d\uparrow}n_{d\downarrow} - \frac{1}{2}(n_{d\uparrow} + n_{d\downarrow})]]] \tag{20}$$

After the decoupling of $\mathcal{H}^i$ by the transformation Eq. (10)

$$\exp[-\Delta\tau\mathcal{H}^i] = \frac{1}{2}\sum_{s=\pm1}\exp[\lambda s(n_{d\uparrow} - n_{d\downarrow})] \ , \ \cosh(\lambda) \equiv \exp(\Delta\tau U/2) \tag{21}$$

and after inserting Eq. (21) into Eq. (20), the partition function $Z^{\Delta\tau}$ is reduced to:

$$Z = \mathrm{Tr}\prod_{l=1}^{L} e^{-\Delta\tau\mathcal{H}^0}\frac{1}{2}\sum_{s_l=\pm1}\exp[\lambda s_l(n_{d\uparrow} - n_{d\downarrow})] = \tag{22}$$

$$= Tr\prod_{l=1}^{L}\frac{1}{2}\sum_{s_l=\pm1} e^{-\Delta\tau\mathcal{H}^0_\uparrow}\exp[\lambda s_l n_{d\uparrow}]e^{-\Delta\tau\mathcal{H}^0_\downarrow}\exp[-\lambda s_l n_{d\uparrow}] = \tag{23}$$

$$= \sum_{s_1 s_2 ... s_L=\pm1} Tr\prod_{l=1}^{L}\frac{1}{2}e^{-\Delta\tau\mathcal{H}^0_\uparrow}\exp[\lambda s_l n_{d\uparrow}]e^{-\Delta\tau\mathcal{H}^0_\downarrow}\exp[-\lambda s_l n_{d\uparrow}] \tag{24}$$

$$Z = \frac{1}{2^L}\sum_{s_1 s_2 ... s_L=\pm1} Tr\prod_{\sigma=\pm1}\prod_{l=1}^{L} Z_l^{\Delta\tau}(\sigma) = \sum_{s_1 s_2 ... s_L=\pm1} Z_{s_1,...,s_L} \tag{25}$$

with

$$Z_l^{\Delta\tau}(\sigma) \equiv D_l(\sigma) = e^{-\Delta\tau\mathcal{H}^0_\sigma}e^{V^\sigma(s_l)} = e^{-\Delta\tau c_i^+ K_{ij} c_j}e^{c_i^+ V^\sigma(s_l)c_i} \tag{26}$$

here sum over repeated indexes is assumed!

In Eq. (26), the $n_s \times n_s$ matrix $V^\sigma(s)$ is diagonal with

$$e^{V^\sigma(s)} = \begin{pmatrix} e^{\lambda\sigma s} & . & . & 0 \\ . & 1 & . & . \\ . & . & 1 & . \\ 0 & . & . & 1 \end{pmatrix} \tag{27}$$

Let us introduce now the following matrix $B_l(\sigma) = e^{-\Delta\tau K} e^{V^\sigma(s_l)}$. Using this definition we can write the partition function as

$$Z = \sum_{s_1 s_2 \ldots s_L = \pm 1} \prod_{\sigma=\pm 1} \det[I + B_L(\sigma) B_{L-1}(\sigma) \ldots B_1(\sigma)] \equiv \sum_{s_1 s_2 \ldots s_L = \pm 1} \det \mathcal{O}_{s_1,\ldots,s_L}(\uparrow) \det \mathcal{O}_{s_1,\ldots,s_L}(\downarrow) \quad (28)$$

where $\mathcal{O}_{s_1,\ldots,s_L}(\sigma)$ the $n_s L \times n_s L$ matrix

$$\mathcal{O}_{s_1,\ldots,s_L(\sigma)} = \begin{pmatrix} 1 & 0 & . & 0 & B_L(\sigma) \\ -B_1(\sigma) & 1 & . & . & 0 \\ 0 & -B_2(\sigma) & 1 & . & . \\ . & . & . & 1 & 0 \\ . & . & . & -B_{L-1}(\sigma) & 1 \end{pmatrix}, \quad (29)$$

As you see $\mathcal{O}$ has been written as an $L \times L$ matrix of $n_s \times n_s$ matrices [$\mathcal{O} \equiv \mathcal{O}_{\{i_l, i_s\}, \{i'_l, i'_s\}}$ with $i_l = 1, \ldots L$ and $i_s = 1, \ldots n_s$].

Now we need to show two things. Let us start with the easier one, we should prove equation 28, or in another words that

$$Tr \prod_{l=1}^{L} Z_l^{\Delta\tau}(\sigma) = Tr \prod_{l=1}^{L} e^{-\Delta\tau c_i^+ K_{ij} c_j} e^{c_i^+ V^\sigma(s_l) c_j} = \det[I + B_L(\sigma) B_{L-1}(\sigma) \ldots B_1(\sigma)]$$

here we droped spin symbol σ.

To prove this one should first prove simplier identity:

$$Tr_{c_i^+, c_i} \{ e^{-c_i^+ A_{i\,j} c_j} e^{-c_i^+ B_{i\,j} c_j} \} \equiv \det[1 + e^{-A} e^{-B}], \quad (30)$$

which can follow from another identity:

$$Tr_{c_i^+, c_i} \{ e^{-c_i^+ A_{i\,j} c_j} e^{-\sum_{i\,j} c_i^+ B_{i\,j} c_j} \} \equiv Tr_{c_i^+, c_i} \{ e^{-\sum_\nu c_\nu^+ l_\nu c_\nu} \}, \quad (31)$$

where $\lambda_\nu = e^{-l_v}$ are the eigenvalues of the matrix $e^{-A} e^{-B}$. From the last identity equation (30) follows immeadiately:

$$Tr_{c_i^+, c_i} \{ e^{-\sum_\nu c_\nu^+ l_\nu c_\nu} \} = Tr \prod_\nu (1 + e^{-l_v}) = \det(1 + e^{-A} e^{-B}).$$

HOME WORK 1: *Prove the identity:* $\det \mathcal{O}_{s_1,\ldots,s_L}(\sigma) \equiv \det[I + B_L(\sigma) B_{L-1}(\sigma) \ldots B_1(\sigma)]$.

□Tip to HM1: The equivalence of $\det O_{s_1,\ldots,s_L}$ with the BSS formula Eq. (59) can then be shown by Gaussian elimination (replacing successively the first row of O by multiples of rows $L, L-1, \ldots, 1$, $\{O_{1i}\}_{i=1,\ldots,L} \to \{O_{1i} - B_L B_{L-1} \ldots B_{L-k+1} \times O_{L-k+1,i}\}_{i=1,\ldots,L}$ for $k = 0, 1, \ldots, L-1$). ■

HOME WORK 2: *Prove the identity* **(31).**

Now we are ready to obtain time-dependent correlation functions (Green functions). It is done by inserting the fermion operators to corresponding time slices equation (25). I would like to point out a few things. First of all, one should clearly understand what kind of GF is used. The natural definition of GF would be (see (25)):

$$\langle\langle A_i B_j \rangle\rangle = \frac{\sum_{s_1 s_2 \ldots s_L = \pm 1} Tr A_i B_j \prod_{\sigma=\pm 1} \prod_{l=1}^{L} Z_l^{\Delta\tau}(\sigma)}{Z} = \frac{\sum_{s_1 s_2 \ldots s_L = \pm 1} \langle A_i B_j \rangle \prod_{\sigma=\pm 1} \det O(\sigma)}{Z} \quad (32)$$

where

$$\langle A_i B_j \rangle = \frac{Tr A_i B_j \prod_{l=1}^{L} Z_l^{\Delta\tau}(\sigma)}{\prod\limits_{\sigma=\pm 1} \det O(\sigma)} = g^{\Delta\tau}_{s_1,\ldots,s_L}|_{i,j}. \tag{33}$$

Note *(very important)*: **Mainly, in the QMC simulations we work with GF** $\langle A_i B_j \rangle = g^{\Delta\tau}_{s_1,\ldots,s_L}|_{i,j}$ $=G_\sigma(s_1,\ldots,s_L)$ (cf (15)), **which is GF for a particular set of auxilary Ising spins.**

$$g^{\Delta\tau}_{s_1,\ldots,s_L}(\tau_{l_1},\tau_{l_2})|_{p_1,p_2} \equiv < a_{p_1}(\tau_{l_1}) a^+_{p_2}(\tau_{l_2}) >= \tag{34}$$

$$= \frac{Tr D_L D_{L-1} \ldots D_{l_1+1} a_{p_1} D_{l_1} \ldots D_{l_2+1} a^+_{p_2} D_{l_2} \ldots D_1}{Tr D_L \ldots D_1} \quad = \tag{35}$$

$$= \frac{Tr D_{l_2} \ldots D_1 D_L \ldots D_{l_2+1} [(D_{l_1} D_{l_1-1} \ldots D_{l_2+1})^{-1} a_{p_1} D_{l_1} \ldots D_{l_2+1}] a^+_{p_2}}{Tr D_{l_2} \ldots D_1 D_L \ldots D_{l_2+1}} \tag{36}$$

where (for $l_1 > l_2$),and similarly one can get expression for $l_1 < l_2$ case.

Using the following identity:

$$a_i D_l = D_l (B_l)_{ij} a_j, \tag{37}$$

we immediately obtain (one should apply a_i to the right and then we get $[(D_{l_1} D_{l_1-1} \ldots D_{l_2+1})^{-1} D_{l_1} \ldots D_{l_2+1}] = 1$ and $\sum_k (B_{l_1} B_{l_1-1\ldots} B_{l_2+1})_{p1,k} a_k$:

$$[(D_{l_1} D_{l_1-1} \ldots D_{l_2+1})^{-1} a_{p_1} D_{l_1} \ldots D_{l_2+1}] = \sum_k (B_{l_1} B_{l_1-1\ldots} B_{l_2+1})_{p1,k} a_k \tag{38}$$

HOME WORK 3: *Prove the identity (***37).**

Now we can inset equation (38) into (34) to get:

$$g^{\Delta\tau}_{s_1,\ldots,s}(\tau_{l_1},\tau_{l_2})|_{p_1,p_2} = \sum_k (B_{l_1} B_{l_1-1\ldots} B_{l_2+1})_{p1,k} \frac{Tr D_{l_2} \ldots D_1 D_L \ldots D_{l_2+1}\, a_k a^+_{p_2}}{Tr D_{l_2} \ldots D_1 D_L \ldots D_{l_2+1}}, \tag{39}$$

and using normal modes of fermion operators we finnaly get representation for the GF $g^{\Delta\tau}_{s_1,\ldots,s}(\tau_{l_1},\tau_{l_2})|_{p_1,p_2}$:

$$< a_{p_1}(\tau_{l_1}) a^+_{p_2}(\tau_{l_2}) >= \left[B_{l_1} B_{l_1-1\ldots} B_{l_2+1} \frac{1}{1 + B_{l_2} \ldots B_1 B_L \ldots B_{l_2+1}} \right]_{p_1,p_2}. \tag{40}$$

Here we have used the following. Let us leave time dependence, then using the identity (31) and defining new fermion operators

$$a_\nu = \sum_i < \nu | i > a_i$$

$$a^+_\nu = \sum_i < i | \nu > a^+_i$$

we can write

$$\langle a_i a_j^+ \rangle = \frac{Tr a_i a_j^+ \prod_\nu e^{-a_\nu l_\nu a_\nu^+}}{\prod_\nu (1+e^{-l_\nu})} =$$
$$= \sum_{\nu'} < \nu' | i >< j | \nu' > \frac{Tr a_{\nu'} a_{\nu'}^+ \prod_\nu e^{-a_\nu l_\nu a_\nu^+}}{\prod_\nu (1+e^{-l_\nu})} =$$
$$= \sum_{\nu'} < \nu' | i >< j | \nu' > \frac{1}{(1+e^{-l_{\nu'}})} =$$
$$= \left[\frac{1}{1+B_L B_{L-1} ... B_1} \right].$$

In absolute analogy we adopted this procedure to formula (40).

It is important to understand that the object $g^{\Delta\tau}$ will be obtained essentially exactly: the only systematic error of the QMC method will consist in the replacement of $\exp(-\Delta\tau H)$ by D_l as an evolution operator between time slices. We are then ultimately interested in the $d-$site Green's function, which we denote by a capital letter $G^{\Delta\tau}(\tau_{l_1}, \tau_{l_2}) \equiv g^{\Delta\tau}_{s_1,...,s}(\tau_{l_1}, \tau_{l_2})|_{1,1}(\tau_{l_1}, \tau_{l_2})$.

Now we can recall out $\mathcal{O}$ matrix which is related to the discretized Ising-spin dependent Green's function by the identity:

$$g^{\Delta\tau}_{s_1,...,s_L} = \mathcal{O}^{-1}_{s_1,...,s_L} \tag{41}$$

$\square$The identity $g^{\Delta\tau}_{s_1,...,s_L} = O^{-1}_{s_1,...,s_L}$ is easily established. It is quite useful to consider the simple example of a 3×3 matrix (of matrices B_i), for which we explicitly write down the inverse.

$$\mathcal{O} = \begin{pmatrix} 1 & 0 & B_3 \\ -B_1 & 1 & 0 \\ 0 & -B_2 & 1 \end{pmatrix} \tag{42}$$

$$\mathcal{O}^{-1} = \begin{pmatrix} \{1+B_3B_2B_1\}^{-1} & -B_3B_2\{1+B_1B_3B_2\}^{-1} & -B_3\{1+B_2B_1B_3\}^{-1} \\ B_1\{1+B_3B_2B_1\}^{-1} & \{1+B_1B_3B_2\}^{-1} & -B_1B_3\{1+B_2B_1B_3\}^{-1} \\ B_2B_1\{1+B_3B_2B_1\}^{-1} & B_2\{1+B_1B_3B_2\}^{-1} & \{1+B_2B_1B_3\}^{-1} \end{pmatrix} \tag{43}$$

The reader will easily be able to verify Eq. (43) and to generalize it for arbitrary L. Manifestly, Eq. (43) reproduces Eq. (40).$\blacksquare$

Now we can calculate (in principle) everything! Let us understand what we can do in practice.

The matrix $\mathcal{O}_{s_1,...,s_L}$ is large (of size $n_s L \times n_s L$), but it need not be manipulated explicitly, as will be shown below.

The crucial fact noted by **Hirsch** and **Fye** is that the Green's functions for two different Ising spin configurations, $(s_1, \ldots, s_L)$ and $(s'_1, \ldots, s'_L)$ are related to each other by a Dyson equation .

Abbreviating $g \equiv g^{\Delta\tau}_{s_1,...,s_L}$ and $g' \equiv g^{\Delta\tau}_{s'_1,...,s'_L}$, *etc*, this Dyson equation reads:

$$g' = g + (g-1)(e^{V'-V} - 1)g' \tag{44}$$

To derive the Dyson equation it is useful to consider the matrix $\mathcal{O}\exp(-V)$ with the $Ln_s \times Ln_s$ matrix

$$e^{-\tilde{V}}_{s_1,...,s_L} = \begin{pmatrix} e^{-V(s_1)} & . & . & 0 \\ . & e^{-V(s_2)} & . & . \\ . & . & . & . \\ 0 & . & . & e^{-V(s_L)} \end{pmatrix} \tag{45}$$

$\mathcal{O}\exp(-\tilde{V})$ is therefore a matrix which depends on $(s_1,\ldots,s_L)$ only in the space- and time-diagonal elements

$$\mathcal{O}_{s_1,\ldots,s_L} e^{-\tilde{V}}_{s_1,\ldots,s_L} - \mathcal{O}_{s'_1,\ldots,s'_L} e^{-\tilde{V}}_{s'_1,\ldots,s'_L} = e^{-\tilde{V}}_{s_1,\ldots,s_L} - e^{-\tilde{V}}_{s'_1,\ldots,s'_L} \tag{46}$$

Abbreviating $g \equiv g_{s_1,\ldots,s_L}$ and $g' \equiv g_{s'_1,\ldots,s'_L}$, *etc*, and using $\mathcal{O} = g^{-1}$, we show that Eq. (46) leads to $\exp(V'-V)g' - g = g[\exp(V'-V)-1]g'$ which is equivalent to Eq. (44).

Derivation:

$\square$ $Oe^V - O'e^{V'} = e^V - e^{V'} \rightarrow (g)^{-1}e^V - (g')^{-1}e^{V'} = e^V - e^{V'} \rightarrow e^V - g(g')^{-1}e^{V'} = ge^V - ge^{V'} \rightarrow$
$e^{V-V'} - g(g')^{-1} = ge^{V-V'} - g \rightarrow e^{V-V'}g' - g = ge^{V-V'}g' - gg' \rightarrow e^{V-V'}g' - g = g[e^{V-V'}-1]g'$■

The Dyson equation brings us back to the description of the impurity problem given in paragraph (III A). In fact, Eq. (44) relates two Green's functions g and g' *via* a projection operator on the d-site, namely $[\exp(V'-V)-1]$:

$$[\exp(V'-V)-1]_{\{i_l,i_s\},\{i'_l,i'_s\}} \propto \delta_{i_l,i'_l}\delta_{i_s,1}\delta_{i'_s,1} \tag{47}$$

The presence of this projection operator translates the possibility to integrate out the conduction band. As a consequence, the Dyson equation Eq. (44) directly relates the Green's functions on the d-site one to another, and this equation remains equally valid in the subspace $i_s = 1, i'_s = 1$. Hence, the $d-$site Green's functions $G^{\Delta\tau}_{s_1,\ldots,s_L}$ also satisfy:

$$G' = G + (G-1)(e^{V'-V})G' \tag{48}$$

viewed as an $L\times L$ matrix equation. As a first application of this Dyson equation, we use it to derive Eq. (13), which follows by putting $G' \equiv G_{(s_1,\ldots,s_L)}, G \equiv \mathcal{G}_0$ - notice that the Dyson equation allows arbitrary values for the auxiliary spins s_i.

Rearranging Eq. (44), it is straightforward to see that $G_{s'_1,\ldots,s'_L}$ for an Ising configuration $(s'_1,\ldots,s'_L)$ can be obtained from $G_{s_1,\ldots,s_L}$ by inversion of an $L\times L$ matrix $\mathcal{A}$, defined in the following equation

$$\mathcal{A}G' = G \ , \ \mathcal{A} \equiv 1 + (1-G)[e^{V'-V}-1] \quad \text{(any two configurations)} \tag{49}$$

to prove this we use Dyson equation(48):

$\square(1+(1-G)[e^{V'-V}-1])G' \rightarrow (1-(G-1)[e^{V'-V}-1])G' \rightarrow G' + G - G' = G$■

In the special case in which $(s'_1,\ldots,s'_L)$ differs from $(s_1,\ldots,s_L)$ by the value of a single spin, say s_l, $\mathcal{A}$ takes on a special form

$$\mathcal{A} = \begin{pmatrix} 1 & 0 & \mathcal{A}_{1\,l} & 0 & . \\ 0 & 1 & \mathcal{A}_{2\,l} & . & . \\ . & 0 & \mathcal{A}_{l\,l} & . & . \\ . & . & . & 1 & 0 \\ . & . & \mathcal{A}_{L\,l} & 0 & 1 \end{pmatrix} \tag{50}$$

Let us understand why it is so. If only one spin differs than all elements of the matrix $[e^{V'-V}-1] = 0$, except one which is $e^{V'(s_l)-V(s_l)}$. It means that $[e^{V'-V}-1]$ matrix has the form:

$$[e^{V'-V}-1] = \begin{pmatrix} 0 & 0 & ... & 0 & . \\ 0 & 0 & ... & . & . \\ . & 0 & e^{V'-V}-1 & . & . \\ . & . & . & 0 & 0 \\ . & . & ... & 0 & 0 \end{pmatrix}$$

$1 + [e^{V'-V}-1] - G[e^{V'-V}-1] = 1 + (1-G)[e^{V'-V}-1] = 1 + (\widetilde{G})[e^{V'-V}-1]$

$$\begin{pmatrix} 1 & 0 & ... & . & . \\ 0 & 1 & ... & . & . \\ . & 0 & 1 & . & . \\ . & . & . & 1 & 0 \\ . & . & ... & 0 & 1 \end{pmatrix} + \begin{pmatrix} \widetilde{G}_{11} & \widetilde{G}_{12} & . & . & \widetilde{G}_{1N} \\ \widetilde{G}_{21} & \widetilde{G}_{22} & . & . & . \\ . & \widetilde{G}_{32} & \widetilde{G}_{33} & . & . \\ . & . & . & . & . \\ . & . & ... & . & \widetilde{G}_{NN} \end{pmatrix} \begin{pmatrix} 0 & 0 & ... & 0 & . \\ 0 & 0 & ... & . & . \\ . & 0 & e^{V'-V}-1 & . & . \\ . & . & . & 0 & 0 \\ . & . & ... & 0 & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 & \mathcal{A}_{1\,l} & 0 & . \\ 0 & 1 & \mathcal{A}_{2\,l} & . & . \\ . & 0 & \mathcal{A}_{l\,l} & . & . \\ . & . & . & 1 & 0 \\ . & . & \mathcal{A}_{L\,l} & 0 & 1 \end{pmatrix} !$$

In that case, $\det \mathcal{A} = \mathcal{A}_{l\,l} = 1 + (1 - G_{l\,l})[\exp(V'_l - V_l) - 1]$. Expanding $\mathcal{A}^{-1}$ in minors, it can easily be seen that $(\mathcal{A}^{-1})_{l\,k} = 0$ for $k \neq l$. In that case the equation (49) simplifies to (remember $G' = \mathcal{A}^{-1}G$ and 48)

$$G' = G + (G-1)(e^{V'-V})G' = G + (G-1)(e^{V'-V})\mathcal{A}^{-1}G \Rightarrow$$

$$G'_{l_1\,l_2} = G_{l_1\,l_2} + (G-1)_{l_1\,l} e^{V'_l - V}_{l\,l} (\mathcal{A}_{l\,l})^{-1} G_{l\,l_1\,l_2} \quad \text{(single flip)} \tag{51}$$

which is a special case of a Sherman-Morrison formula. Eq. (51) can also be used to show that

$$\frac{\det \mathcal{O}'}{\det \mathcal{O}} = \frac{\det G}{\det G'} = \det \mathcal{A} = 1 + (1 - G_{l\,l})[\exp(V'_l - V_l) - 1] \tag{52}$$

(Reminder: $\det AB = \det A \det B$. And $O = G^{-1}$)

It is remarkable that all the equations (48 - 52) express *exact* relations between discretized Green's functions $G^{\Delta\tau}$. The only error committed is related to the Trotter break-up (Eq. (26)). We also note that the fermionic sign problem plays no role in any of the calculations. The determinants in Eq.˜(53)generally have the same sign, and their ratio can be interpreted as a ratio of probabilities.

In a Monte Carlo simulation, Ising spin configurations are generated with a probability proportional to $\det \mathcal{O}^{\uparrow} \det \mathcal{O}^{\downarrow}$, and the physical Green's function $G^{\Delta\tau}$ is then given from Eq. (56) as an average of $G^{\Delta\tau}_{s_1,\ldots,s_L}$ with this measure. As usual, there is some freedom in the choice of the Monte Carlo dynamics, which must however satisfy detailed balance:

$$\frac{P(\mathbf{s} \to \mathbf{s}')}{P(\mathbf{s}' \to \mathbf{s})} = \frac{\prod_\sigma \det \mathcal{O}(\sigma)_{\mathbf{s}'}}{\prod_\sigma \det \mathcal{O}(\sigma)_{\mathbf{s}}} \tag{53}$$

Both the heat-bath and the Metropolis dynamics satisfy this condition:

$$P(\mathbf{s} \to \mathbf{s}') = \frac{\prod_\sigma \det \mathcal{O}(\sigma)_{\mathbf{s}'}}{[\prod_\sigma \det \mathcal{O}(\sigma)_{\mathbf{s}'} + \prod_\sigma \det \mathcal{O}(\sigma)_{\mathbf{s}}]} \quad \text{(Heat bath)} \tag{54}$$

$$P(\mathbf{s} \to \mathbf{s}') = \begin{cases} 1 & \text{if } \prod_\sigma \det \mathcal{O}(\sigma)_{\mathbf{s}'} > \prod_\sigma \det \mathcal{O}(\sigma)_{\mathbf{s}} \\ \frac{\prod_\sigma \det \mathcal{O}(\sigma)_{\mathbf{s}'}}{\prod_\sigma \det \mathcal{O}(\sigma)_{\mathbf{s}}} & \text{otherwise} \end{cases} \quad \text{(Metropolis)} \tag{55}$$

In both cases, the transition probability is a function of the *ratio* of determinants, which can be computed easily (*cf* Eq. (52)) with a computational effort of $O(1)$. If the move $s \to s'$ is accepted, $G^{\Delta\tau}_{s_1 \ldots s_L}$ is updated with a computational burden of $O(L^2)$, using Eq. (51). The computational effort is thus large for each *accepted* move only. This fact renders the simulation rather insensitive to the problem of small acceptance probabilities.

C. Implementation of the Hirsch-Fye algorithm

We can now assemble the essential ingredients of the Hirsch-Fye algorithm :

1. The calculation **starts from the Green's function** $G^{\Delta\tau}_{s_1,\ldots,s_L}(\tau_i,\tau_j)$, with all Ising spins formally set to $s_1 = \ldots = s_L = 0$. In the LISA context, $G^{\Delta\tau}_{s_1=0,\ldots,s_L=0}(\tau_i - \tau_j)$ is a discretized version $\mathcal{G}_0^{\Delta\tau}$ of the Weiss function $\mathcal{G}_0$, which generally has been determined in the previous iteration by the self-consistency condition (whose implementation will be discussed shortly). At the first step of the iteration, an initial guess is made for $\mathcal{G}_0^{\Delta\tau}$.

2. The Green's function $G^{\Delta\tau}_{s_1,\ldots,s_L}(\tau_l,\tau_{l'})$ for an arbitrary initial configuration with $s_1 = \pm 1 \ldots s_L = \pm 1$ is calculated by **explicit inversion of the matrix A in Eq. (49).**

3. From then on, configurations are visited using single spin-flips. In that case, Green's functions can be **updated using Eq. (51)** (every so often, one checks that the precision has not degraded by doing a complete update as indicated above).

4. Physical Green's functions $G^{\Delta\tau}(\tau_l - \tau_{l'})$ are determined as averages of the configuration- dependent functions $G^{\Delta\tau}_{s_1,\ldots,s_L}(\tau_l,\tau_{l'})$ with the Ising spin configurations weighted according to Eq. (52).

The physical Green's function is given by (cf (32)):

$$G^{\Delta\tau,\uparrow\downarrow}(\tau_l,\tau_{l'}) = \frac{\sum_{s_1,\ldots,s_L} Z_{s_1,\ldots,s_L} g^{\Delta\tau}_{s_1,\ldots,s}(\tau_l,\tau_{l'})|^{\Delta\tau}_{1,1}(\tau_l,\tau_{l'})}{\sum_{s_1,\ldots,s_L} Z_{s_1,\ldots,s_L}} = \tag{56}$$

$$= -\frac{\sum_{s_1,\ldots,s_L}\prod_{\sigma=\pm1}\det\mathcal{O}(\sigma)_{s_1,\ldots,s_L}\mathcal{O}^{-1}(\uparrow\downarrow)_{s_1,\ldots,s_L}(\tau_l,\tau_{l'})}{\sum_{s_1,\ldots,s_L}\prod_{\sigma=\pm1}\det\mathcal{O}(\sigma)_{s_1,\ldots,s_L}} \tag{57}$$

(in order to be explicit, we have reintroduced the dependence on physical spin in Eq. (56)). If a complete enumeration of Ising spin configurations is possible, the Green's function can be readily evaluated using this formula. It is advisable in this case (Georges and Krauth, 1993) to perform this enumeration using the so-called Gray code, which allows to enumerate all the configurations of the Ising spins *via* single spin flips. The Gray code enumeration of Eq (56) produces *numerically exact* results for $G^{\Delta\tau}$.

Notice also that the physical Green's function $G^{\Delta\tau}$ is translation invariant in time $G^{\Delta\tau}(\tau_i,\tau_j) = G^{\Delta\tau}(\tau_i - \tau_j)$, a property which the Ising-spin dependent quantities $G^{\Delta\tau}_{s_1\ldots s_L}$ lack. This property can be used to reduce statistical noise.

Compared to Blankenbecler, Scalapino and Sugar (BSS) (1981) BSS algorithm, the method of Hirsch and Fye thus not only yields a very natural numerical implementation of the impurity problem which integrates out the conduction band electrons from the beginning (i.e.allows a general Weiss field $\mathcal{G}_0$). It also presents the enormous advantage of being numerically stable at low temperature, and allows to reach temperatures significantly lower than the bandwidth. The remaining

limitations of the Hirsch-Fye algorithm can be described as follows:

- Only imaginary-time (or Matsubara frequency) quantities can be obtained directly. Real-frequency calculations require analytic continuation algorithms (cf. Sec.**??**).

- The lowest temperatures that can be reached are limited by the number of time-slices that one can handle, because the matrices to be multiplied become prohibitively large. On a present-day workstation, the computations with, let's say, 256 time-slices present already a considerable investment in computer time. If the problem at hand is not altogether trivial, we may expect (and notice in fact) that the finite $\Delta\tau$ behavior is intricate, which means that we have to choose $\Delta\tau$ sensibly smaller than 1. Thus, even if U is not too big, the range of accessible temperatures is limited to temperatures of the order of $\beta \simeq 30$ -or smaller- (in the units of the half-bandwidth D). We shall see in the next section that very accurate descriptions of the relevant impurity models are possible, which are much more economical in the number of parameters used (256 in the present example). The condition for this is that one uses an adaptive discretization, which may change with the problem at hand, instead of a fixed grid, as is done in the QMC procedure, in which $\tau_i = i \cdot \Delta\tau$.

IV. THE QMC ALGORITHM IN FORTRAN REALIZATION.

Here we present the floating chart of the QMC program

Input $\mathcal{G}_0(\tau)$ →**Initialization** →
[sub:initial]

Start QMC simulations →
1) make spin flip : [sub : detrat] : (52)
2) Metropolis ot heat bath : (53)
if (flip_accepted) : [sub : record] : (51)
3) GF calculation : (49)
4) check degradation : [sub : update]

End QMC simulations →

Output $G(\tau)$

The Hirsch-Fye algorithm is remarkably stable, and a full-size program (such as the program `lisaqmc.f` provided with this article) can be written relatively easily.

In the program `lisaqmc.f`, the different parts of the algorithm are distributed over a few subroutines, in a way explained in the following table:

function	*purpose*	*equation*
`detrat`	calculate determinant ratio	Eq. (52)
`initial`	initialize ($\mathcal{G}_0^{\Delta\tau}(\tau) \to \mathcal{O}^{-1}_{0,\ldots,0}(\tau,\tau')$)	–
`record`	perform fast update	Eq. (51)
`update`	compute $G^{\Delta}_{s_1,\ldots,s_L}$ from $\mathcal{G}_0^{\Delta}$	Eq. (49)

Besides the Monte Carlo update, the program `lisaqmc.f` also allows one to compute physical Green's functions by *complete enumeration* using the Gray code. In this method, *all* possible configurations of Ising spins are visited in an order in which every configuration of spins $(s_1,\ldots,s_L)$ differs from the following one $(s'_1,\ldots,s'_L)$ in a single index only ($s_i = s'_i$, except for a single value of i). More precisely, the configurations are enumerated by making a single spin-flip on the larger possible index i (without going back to a previously visited configuration). As an example, let us give the first steps of a Gray code enumeration for $L = 5$:

$$\begin{array}{cc}
\begin{bmatrix} + & + & + & + & + \\ + & + & + & + & - \\ + & + & + & - & - \\ + & + & + & - & + \\ + & + & - & - & + \\ + & + & - & - & - \\ + & + & - & + & - \\ + & + & - & + & + \\ & & \vdots & & \end{bmatrix} & \begin{bmatrix} + & + & + & + & + \\ + & + & + & + & - \\ + & + & + & - & + \\ + & + & + & - & - \\ + & + & - & + & + \\ + & + & - & + & - \\ + & + & - & - & + \\ + & + & - & - & - \\ & & \vdots & & \end{bmatrix} \\
\text{Gray Code} & \text{standard}
\end{array} \tag{58}$$

This algorithm can be simply programmed (*cf* Press *et al* 1991). By doing this, we can again compute the Green's function $G^{\Delta}_{s_1,\ldots,s'_k,\ldots s_L}$ from $G^{\Delta}_{s_1,\ldots,s_k,\ldots s_L}$ by the fast update `record` (in $O(L^2)$ steps), rather

than having to compute it from $\mathcal{G}_0^{\Delta}$ in $O(L^3)$ steps (using `update`). Naturally, the averages must now be computed by including the determinant in the statistical weight. Furthermore, the normalization need also be calculated. Further details can be found in the program `lisaqmc.f`.

Both the Monte Carlo and the exact enumeration include checks to avoid loss of precision. In the Monte Carlo algorithm, this is done from time to time by confronting the result of subroutine `update` with the single spin-flip updates. In the exact enumeration calculation, the precision can be evaluated simply by restarting the Gray code with an initial spin configuration $(s_1, \ldots, s_L)$ different from $(1, \ldots, 1)$.

V. RELATIONSHIP WITH OTHER QMC ALGORITHMS

Historically, the first applications of Quantum Monte Carlo methods to impurity models did not use the Hirsch-Fye algorithm, but the original method for performing QMC calculations for lattice fermions, which is due to Blankenbecler, Scalapino and Sugar (BSS) (1981). The two methods are very closely related: The BSS algorithm simply computes the determinant of $\mathcal{O}_{s_1,\ldots,s_L}$, in the following way:

$$Z_{s_1,\ldots,s_L} = \prod_{\sigma=\pm 1} \det[1 + B_{s_1}(\sigma)\, B_{s_2}(\sigma) \ldots B_{s_{L-1}}(\sigma)\, B_{s_L}(\sigma)] \equiv \prod_{\sigma=\pm 1} \det W_{s_1,\ldots,s_L}(\sigma). \tag{59}$$

Similarly, discretized Green's functions can also be expressed in terms of the matrices B_i:

$$G^{\Delta\tau}_{s_1,\ldots,s_L}(\tau_l, \tau_{l'}) = [B_{s_l} B_{s_{l-1}} \ldots B_{s_{l'+1}} \frac{1}{1 + B_{s'_l} \ldots B_{s_1} B_{s_L} \ldots B_{s_{l'+1}}}]_{1,1} \quad (l \geq l') \tag{60}$$

(BSS, 1981 for $l < l'$). The matrices appearing in Eq. (59) and (60) are of size $n_s \times n_s$, independently of the number of time-slices, and the determinant of $W_{s_1,\ldots,s_L}$ can be computed explicitly. Notice that in this formulation $W_{s_1,\ldots,s_L}$ is a $n_s \times n_s$ matrix, and the number of time-slices is reflected solely in the number of matrices which appear in the products of Eqs (59) and (60). Unfortunately, the product of matrices $B_{s_1}(\sigma)\, B_{s_2}(\sigma) \ldots B_{s_{L-1}}(\sigma)\, B_{s_L}(\sigma)$ is usually very badly conditioned. This generates numerical instabilities which render the calculation of $\det(W_{s_1,\ldots,s_L})$ difficult in practice. As a result of the severe numerical instabilities, the early attempts to treat the single impurity problem with QMC methods (Gubernatis *et al.* 1986), which used the BSS algorithm, have met with little success. Note however that the more recent 'balancing schemes' for the BSS algorithm (Sugiyama and Koonin, 1986, White *et al*, 1989) have to our knowledge not been applied to impurity models, and could lead to an important improvement.

In order to avoid misunderstandings, we clarify the following: usual (finite-dimensional) QMC calculations, which apply the BSS algorithm, are haunted by two completely unrelated problems: the bad conditioning of the product of matrices $B_{s_1}(\sigma) \cdots B_{s_L}(\sigma)$, and by the fermionic sign problem ($\det(W_{s_1,\ldots,s_L})$ may not always have the same sign). In impurity problems, one usually encounters neither of these problems, since one is able to use a stable algorithm (Hirsch-Fye), and since the fermionic sign problem is empirically found to play no role. There are techniques - 'balancing schemes' which attempt to solve the problem of the numerical instability.