HOW TO WRITE A DETERMINANT QMC CODE

Introduction

I am going to invert the usual order of teaching. These notes will *begin* with the prescription for writing a determinant QMC code for the Hubbard model. *After* I describe how to do it, I go through some of the derivations!

The Hamiltonian

Our goal is to write a QMC code for the Hubbard Hamiltonian,

$$\begin{aligned} \hat{H} &= \hat{K} + \hat{V} \\ \hat{K} &= -\sum_{ij\sigma} t_{ij} \left(c^{\dagger}_{i\sigma} c_{j\sigma} + c^{\dagger}_{j\sigma} c_{i\sigma} \right) - \mu \sum_{i\sigma} n_{i\sigma} \\ \hat{V} &= U \sum_{i} (n_{i\uparrow} - \frac{1}{2})(n_{i\downarrow} - \frac{1}{2}) \end{aligned} \tag{1}$$

The indices i and j run from 1 to the number of spatial sites N of the lattice.

Besides the Hamiltonian $\hat{H}$, the physics is also determined by the inverse temperature $\beta = 1/T$. We are going to divide β into L 'imaginary time intervals', $\beta = L\,\Delta\tau$. The length of each interval $\Delta\tau$ should be chosen such that $t\,U\,(\Delta\tau)^2 < 1/10$.

The Kinetic Energy Matrix

The kinetic energy matrix contains all the terms in the Hamiltonian which are quadratic in the fermion creation and destruction operators. That is, we write,

$$\hat{K} = \sum_{\sigma} \begin{pmatrix} c^{\dagger}_{1\sigma} & c^{\dagger}_{2\sigma} & \cdots \end{pmatrix} \begin{pmatrix} k_{11} & k_{12} & \cdots \\ k_{21} & k_{22} & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix} \begin{pmatrix} c_{1\sigma} \\ c_{2\sigma} \\ \vdots \end{pmatrix}. \tag{2}$$

k is defined to be the NxN matrix with elements $\Delta\tau k_{ij}$.

As an example, for a one dimensional Hubbard model with $N = 6$ sites, nearest neighbor hopping, and periodic boundary conditions,

$$k = \Delta\tau \begin{pmatrix} -\mu & -t & 0 & 0 & 0 & -t \\ -t & -\mu & -t & 0 & 0 & 0 \\ 0 & -t & -\mu & -t & 0 & 0 \\ 0 & 0 & -t & -\mu & -t & 0 \\ 0 & 0 & 0 & -t & -\mu & -t \\ -t & 0 & 0 & 0 & -t & -\mu \end{pmatrix} \tag{3}$$

The Interaction Energy Matrix

Fill an array $s(i,l)$ (the 'Hubbard-Stratonovich field') randomly with values ± 1. The first index i goes from 1 to N, and the second index l goes from 1 to L. Define a set of L

diagonal matrices, each of dimension N,

$$v_\uparrow(l) = \lambda \begin{pmatrix} s(1,l) & 0 & 0 & 0 & \cdots \\ 0 & s(2,l) & 0 & 0 & \cdots \\ 0 & 0 & s(3,l) & 0 & \cdots \\ 0 & 0 & 0 & s(4,l) & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix} \tag{4}$$

Here the parameter λ is given by $\cosh \lambda = e^{U\Delta\tau/2}$. The matrices for the down spin electrons differ only by a sign: $v_\downarrow(l) = -v_\uparrow(l)$.

Initializing The Greens Function

Compute the up and down Green's functions,

$$G_\sigma = [\ I + e^k\, e^{v_\sigma(1)}\, e^k\, e^{v_\sigma(2)}\, e^k\, e^{v_\sigma(3)} \cdots\ e^k\, e^{v_\sigma(L)}\ ]^{-1} \tag{5}$$

Here I is the N dimensional identity matrix.

Updating the Hubbard-Stratonovich Field

Suggest a change in the Hubbard Stratonovich field on site $i = 1$ of imaginary time slice $l = L$ by computing the quantity,

$$\begin{aligned} d_\uparrow &= 1 + (\,1 - [G_\uparrow]_{ii}\,)\,(\,e^{-2\lambda\, s(i,l)} - 1\,) \\ d_\downarrow &= 1 + (\,1 - [G_\downarrow]_{ii}\,)\,(\,e^{+2\lambda\, s(i,l)} - 1\,) \\ d &= d_\uparrow d_\downarrow \end{aligned} \tag{6}$$

Throw a uniformly distributed random number, $0 < r < 1$. If $r < d$, update the Hubbard Stratonovich field on site i of imaginary time slice l via $s(i,l) = -s(i,l)$.

Updating the Greens Function

If the move was accepted, the Green's functions, which depend on s (see Eq. 5 and remember $v_\sigma(l)$ are functions of s) will now be different. You could recompute G_σ from Eq. 5, using the new s. This will take a time which goes as N^3, since it involves a matrix inversion. There's a faster (order N^2) trick to get the new G_σ, which takes advantage of the fact that only one element in one of the $v_\sigma(l)$ has changed. Compute the vectors,

$$\begin{aligned} c_{j\uparrow} &= -(\,e^{-2\lambda\, s(i,l)} - 1\,)\,[G_\uparrow]_{ij} + \delta_{ji}\,(\,e^{-2\lambda\, s(i,l)} - 1\,) \\ c_{j\downarrow} &= -(\,e^{+2\lambda\, s(i,l)} - 1\,)\,[G_\downarrow]_{ij} + \delta_{ji}\,(\,e^{+2\lambda\, s(i,l)} - 1\,) \\ b_{k\uparrow} &= [G_\uparrow]_{ki}\ /\ (\,1 + c_{i\uparrow}\,) \\ b_{k\downarrow} &= [G_\downarrow]_{ki}\ /\ (\,1 + c_{i\downarrow}\,) \end{aligned} \tag{7}$$

Here δ_{ij} is the usual Kronecker δ. Remember that i is the fixed site whose Hubbard-Stratonovich field is being updated. The free indices j, k run from 1 to N. Then the new G_σ are given by

$$[G_\sigma]_{jk} = [G_\sigma]_{jk} - b_{j\sigma}\, c_{k\sigma}. \tag{8}$$

Don't forget to update your interaction energy matrix if you accept the move (Eq. 4). After the new G_σ are computed, go to Hubbard-Statonovich field on the second spatial site on imaginary time slice $l = L$ and suggest a change to it, and follow the procedure of Eqs. 6-8 again, with $i = 2$. Continue this until all spatial sites of time slice $l = L$ are updated.

Wrapping the Greens Function

After all spatial sites i of imaginary time slice $l = L$ have been updated, change the Green's functions via,

$$G_\sigma = [\, e^k \, e^{v_\sigma(l)} \,] \; G_\sigma \; [\, e^k \, e^{v_\sigma(l)} \,]^{-1} \tag{9}$$

Now update all the Hubbard-Stratonovich variables on imaginary time slice $l = L - 1$ following the procedures of Eqs. 6-8. When all spatial sites of imaginary time slice are finished, wrap the Greens functions using Eq. 9 again.

Continue the process of Eqs. 6-9 until all imaginary time slices are updated.

Measurements

After completing an entire set of updates to all the space-time points of the lattice. make measurements. For example, the density of electrons of spin σ on site i is given by,

$$\langle n_{i\sigma} \rangle = 1 - [G_\sigma]_{ii}. \tag{10}$$

The double occupancy rate on site i is

$$\langle n_{i\uparrow} n_{i\downarrow} \rangle = (\, 1 - [G_\uparrow]_{ii} \,) \; (\, 1 - [G_\downarrow]_{ii} \,) \tag{11}$$

The local moment on site i is,

$$\langle (n_{i\uparrow} - n_{i\downarrow})^2 \rangle = \langle n_{i\uparrow} + n_{i\downarrow} \rangle - 2 \langle n_{i\uparrow} n_{i\downarrow} \rangle. \tag{12}$$

The correlation between moments on sites i and j, for $i \neq j$, is given by,

$$\begin{aligned} S_{+i} &= c^\dagger_{i\uparrow} c_{i\downarrow} \\ S_{-j} &= c^\dagger_{j\downarrow} c_{j\uparrow} \\ \langle S_{+i} S_{-j} \rangle &= -[G_\uparrow]_{ji} \; [G_\downarrow]_{ij} \end{aligned} \tag{13}$$

You can also measure pairing correlations, charge density wave correlations, etc.

Full Monte Carlo

Begin by initializing the Hubbard-Stratonovich field and computing the Kinetic and Interaction matrices (Eqs. 3,4), and finally the Green's function (Eq. 5). Do a few hundred 'equilibration' sweeps of the lattice (Eqs. 6-9) *without* making any measurements. Follow this by a few thousand 'measurement' sweeps in which you perform the operations of Eqs. 6-9 and also Eqs. 10-12. Normalize your measurements to the number of measurement sweeps performed.

Congratulations, you're done!

We will now discuss the background of the procedure which we have just described.

DERIVATION

A Useful Analogy: Multidimensional Gaussian Integration

The equations involved in determinant QMC bear many similarities with multidimensional Gaussian integrals. Reviewing these identities will help provide an intuitive feel for the formulae of determinant QMC, within a familiar context.

The generalization of the one dimensional Gaussian integral,

$$\int_{-\infty}^{+\infty} dx\, e^{-ax^2} = \frac{\sqrt{\pi}}{a}, \tag{14}$$

to many dimensions is,

$$Z = \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \ldots \int_{-\infty}^{+\infty} dx_1 dx_2 \ldots dx_N \; e^{-\vec{x}\, A\, \vec{x}^T} = \frac{\pi^{n/2}}{\sqrt{\det A}}. \tag{15}$$

Here $\vec{x}$ is an N dimensional vector of real numbers and A is a real, symmetric, N dimensional matrix. I have used the notation Z for the integral to emphasize that it would be the partition function for a set of classical variables whose action is given by the quadratic form $\vec{x} A \vec{x}^T$.

We also know how to do these integrals when the integrand includes factors of x_i.

$$\langle x_i x_j \rangle = Z^{-1} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \ldots \int_{-\infty}^{+\infty} dx_1 dx_2 \ldots dx_N \; x_i x_j \; e^{-\vec{x}\, A\, \vec{x}^T} = \frac{1}{2}[A^{-1}]_{ij} \tag{16}$$

Again, the notation $\langle x_i x_j \rangle$ emphasizes a possible statistical mechanical interpretation of the ratio of integrals.

Further factors of x_i in the integrand generate expressions like,

$$\begin{aligned} \langle x_i x_j x_k x_l \rangle &= Z^{-1} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \ldots \int_{-\infty}^{+\infty} dx_1 dx_2 \ldots dx_N x_i x_j x_k x_l e^{-\vec{x} A \vec{x}^T} \\ &= \frac{1}{4}([A^{-1}]_{ij}[A^{-1}]_{kl} + [A^{-1}]_{ik}[A^{-1}]_{jl} + [A^{-1}]_{il}[A^{-1}]_{jk}). \end{aligned} \tag{17}$$

These are similar in form to 'Wick's Theorem', which tells us that contractions of products of many fermion operators can be expressed as sums of products of contractions taken two operators at a time, in all possible permutations.

While it is possible to do these integrals with arbitrary polynomials as part of the integrand, they cannot be done when a quartic term appears in the exponential. We shall see shortly the analogies of these various statements for traces over fermion Hamiltonians.

Basic Formalism of Determinant QMC

In solving the Hubbard model we want to evaluate expressions like

$$\begin{aligned} \langle \hat{A} \rangle &= Z^{-1} \,\mathrm{Tr}\, [\hat{A} e^{-\beta \hat{H}}] \\ Z &= \mathrm{Tr}\, e^{-\beta \hat{H}} \end{aligned} \tag{18}$$

The "Tr" is a trace over the 4^N dimensional Hilbert space, where N is the number of sites.

In analogy with multidimensional Gaussian integration, we can do such traces if they are over *quadratic* forms of fermion operators. Suppose

$$\hat{H} = \begin{pmatrix} c^\dagger_{1\sigma} & c^\dagger_{2\sigma} & \cdots \end{pmatrix} \begin{pmatrix} h_{11} & h_{12} & \cdots \\ h_{21} & h_{22} & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix} \begin{pmatrix} c_{1\sigma} \\ c_{2\sigma} \cdots \end{pmatrix}. \tag{19}$$

Here h is an NxN matrix. The identity is,

$$Z = \mathrm{Tr}\, e^{-\beta \hat{H}} = \det[I + e^{-\beta h}]. \tag{20}$$

Note that while the original "Tr" is over a quantum mechanical 4^N dimensional Hilbert space, the "det" is a usual determinant of NxN matrices. "I" is the N dimensional identity matrix and "h" is the matrix of *numbers* entering the definition of $\hat{H}$. It is worth emphasizing that because we are taking the trace over the full 4^N dimensional Hilbert space, we are including states of all occupation numbers. The determinant QMC method, as formulated here, works in the grand canonical ensemble. Particle density is controlled by changing the chemical potential.

It is trivial to check that Eq. 20 holds for a single fermion degree of freedom, with Hamiltonian $\hat{H} = \epsilon\, c^\dagger c$. There are two states in the Hilbert space and

$$Z = \langle\, 0 \,|\, e^{-\beta\, \epsilon\, c^\dagger c} \,|\, 0 \rangle + \langle\, 1 \,|\, e^{-\beta\, \epsilon\, c^\dagger c} \,|\, 1 \,\rangle = 1 + e^{-\beta\, \epsilon}. \tag{21}$$

More generally (e.g. for more than one fermion degree of freedom) Eq. 20 can be verified by going to the basis where h is diagonal. The equations can also be derived by employing the techniques of Grassman integration.

There is a more general identity. If one has a *set* of quadratic Hamiltonians $l = 1, 2, \ldots L$

$$\hat{H}(l) = \begin{pmatrix} c^\dagger_{1\sigma} & c^\dagger_{2\sigma} & \cdots \end{pmatrix} \begin{pmatrix} h(l)_{11} & h(l)_{12} & \cdots \\ h(l)_{21} & h(l)_{22} & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix} \begin{pmatrix} c_{1\sigma} \\ c_{2\sigma} \cdots \end{pmatrix}, \tag{22}$$

then,

$$Z = \mathrm{Tr}\,[e^{-\Delta\tau \hat{H}(1)} e^{-\Delta\tau \hat{H}(2)} \cdots e^{-\Delta\tau \hat{H}(L)}] = \det[\, I + e^{-\Delta\tau h(1)} e^{-\Delta\tau h(2)} \cdots e^{-\Delta\tau h(L)}]. \tag{23}$$

Here I have changed the prefactor in the exponential from β to $\Delta\tau$ for reasons which will soon be clear. It is also true that,

$$\begin{aligned} G_{ij} = \langle c_{i\sigma} c^\dagger_{j\sigma} \rangle &= Z^{-1}\, \mathrm{Tr}\,[c_{\,i\sigma} c^\dagger_{j\sigma}\; e^{-\Delta\tau H(1)} e^{-\Delta\tau H(2)} \cdots e^{-\Delta\tau H(L)}\,] \\ &= [\, I + e^{-\Delta\tau h(1)} e^{-\Delta\tau h(2)} \cdots e^{-\Delta\tau h(L)}\,]^{-1}_{ij}. \end{aligned} \tag{24}$$

The "fermions Greens function" is just an appropriate matrix element of the inverse of the NxN matrix whose determinant gives the partition function.

The above formulae describe how to perform traces over quadratic forms of fermion degrees of freedom. Unfortunately, the Hubbard Hamiltonian has an interaction term

$Un_{i\uparrow}n_{i\downarrow} = Uc^\dagger_{i\uparrow}c_{i\uparrow}c^\dagger_{i\downarrow}c_{i\downarrow}$ which is quartic in the fermion operators. To handle such terms, we employ the (discrete) Hubbard–Stratonovich transformation,

$$e^{-U\Delta\tau(n_\uparrow-\frac{1}{2})(n_\downarrow-\frac{1}{2})} = \frac{1}{2}e^{-\frac{U\Delta\tau}{4}}\sum_s e^{\lambda\, s\,(n_\uparrow-n_\downarrow)} \tag{25}$$

Here $\cosh\lambda = e^{U\Delta\tau/2}$, and s is an Ising variable which can take on the two values $S = \pm 1$. This identity can be verified by explicitly enumerating the 4 possible choices for $n_\uparrow, n_\downarrow$.

Now we divide $\beta = L\Delta\tau$ and employ the Trotter decomposition. This allows us to isolate different pieces of the Hamiltonian. We write $\hat{H} = \hat{K}+\hat{V}$ where $\hat{K}$ contains all the one–body pieces and $\hat{V}$ the on–site Hubbard interaction. Then,

$$Z = \mathrm{Tr}\, e^{-\beta\hat{H}} = \mathrm{Tr}\,[e^{-\Delta\tau\hat{H}}]^L \approx \mathrm{Tr}\,[\, e^{-\Delta\tau\hat{K}}\, e^{-\Delta\tau\hat{V}}\, e^{-\Delta\tau\hat{K}}\, e^{-\Delta\tau\hat{V}}\cdots]. \tag{26}$$

The final expression is only approximate since $\hat{K}$ and $\hat{V}$ do not commute. However, the approximation becomes better and better as L increases ($\Delta\tau$ decreases). As mentioned before, the errors should be pretty small if $t\,U\,(\Delta\tau)^2 \approx 1/10$.

The $e^{-\Delta\tau\hat{K}}$ are quadratic in the fermion operators. For each factor of the L terms $e^{-\Delta\tau\hat{V}}$ above, we introduce N Hubbard–Stratonovich fields, one for each of the spatial sites where we have an on–site interaction to decouple. The Hubbard–Stratonovich field $s(i,l)$ therefore has two indices, space i and imaginary–time l. Now the $e^{-\Delta\tau\hat{V}(l)}$ are also quadratic in the fermion operators. We put an argument l on $\hat{V}$ to emphasize that while the $\hat{K}$ are all identical, the $\hat{V}(l)$ contain different Hubbard–Stratonovich fields on the different imaginary time slices.

Applying Eqs. 22-23 allows the analytic evaluation of the trace,

$$Z = \sum_{s(il)} \mathrm{det}M_\uparrow\ \mathrm{det}M_\downarrow, \tag{27}$$

with,

$$M_\sigma = I + e^{-k}e^{-v_\sigma(1)}e^{-k}e^{-v_\sigma(2)}\cdots e^{-k}e^{-v_\sigma(L)}. \tag{28}$$

We get a determinant for each of the two spin species. The quantum partition function has now been expressed to a *classical* monte carlo problem: We need to sum over the possible configurations of the real, classical, variables $s(i,l)$ with the "Boltzmann weight" which is the product of the two fermion determinants. Note that as in world-line QMC, the classical variable to be summed over has an additional index l labeling imaginary time.

Eqs. 2-4 can now be understood as coming from applying the general operator identity of Eqs. 22-23 to our specific problem of evaluating Eq. 26, with the interaction operators $\hat{V}$ made into quadratic forms by using Eq. 25.

The algorithm, as stated, scales in CPU time as N^4L. The reason is that re–evaluating the determinant of M' takes N^3 operations, and we must do that NL times to sweep through all the Hubbard–Stratonovich variables (if, as is typically done, we change just one at a time).

This scaling can be reduced to N^3L. (In what follows I will drop the spin indices.) The idea is to write $M' = M + dM$ and the ratio of determinants as,

$$\mathrm{det}M'/\mathrm{detM} = \mathrm{det}(M^{-1}\,M') = \mathrm{det}(M^{-1}\,(M + dM)) = \mathrm{det}(I + G\,dM), \tag{29}$$

with the definition $G = M^{-1}$. It turns out that dM is very simple because when a Hubbard–Stratonovich field is flipped, a single diagonal entry in $v(l)$ changes. Because dM is sparse, the evaluation of $\mathrm{det}(I + G\,dM)$ takes a cpu time independent of N and L! In fact, a little bit of thought will convince you that Eq. 6 arises from Eq. 31 and the form for dM.

However, we need to know $G = M^{-1}$ for this calculation, and once the Hubbard-Stratonovich field change is made, one needs to update G. This updating G does not take N^3 iterations, as one might expect of a matrix inversion, but can be done in only N^2 operations, again as a result of the simplicity of the change dM. The relevant identity which relates the new $G' = (M + dM)^{-1}$ to the old $G = M^{-1}$ is an application of the "Sherman–Morrison" formula given, for example, in Press's 'Numerical Recipes'. If you work through the Sherman-Morrison formula, as applied to our problem, you end up with Eqs. 7-8.

A final comment concerns the need for 'wrapping' Eq. 9. The use of Eq. 31 to derive Eq. 6, and the Serman-Morrison formula to derive Eqs. 7-8 require that the imaginary time slice of the Hubbard-Stratonovich variable being updated be at the end of the product in Eq. 28. The process of wrapping moves the appropriate interaction matrix to the end of the product through a cyclic permutation. That is,

$$[e^{-k}e^{-v_\sigma(L)}]\;[I + e^{-k}e^{-v_\sigma(1)}e^{-k}e^{-v_\sigma(2)}\cdots e^{-k}e^{-v_\sigma(L)}]^{-1}\;[e^{-k}e^{-v_\sigma(L)}]^{-1} \tag{30}$$

$$= [I + e^{-k}e^{-v_\sigma(L)}e^{-k}e^{-v_\sigma(1)}\cdots e^{-k}e^{-v_\sigma(L-1)}]^{-1} \tag{31}$$

Subtleties and "Tricks of the Trade"

While the above formulae allow you to write a "bare–bones" determinant QMC algorithm, there are a number of refinements which are important.

(1.) It is possible to measure correlation functions with non–zero imaginary time separation, but this requires considerably more work. Analytic continuation of such correlations is required to get the dynamical response. That is quite difficult.

(2.) The product of matrices required in constructing M and hence $G = M^{-1}$ (see Eq. 5 and Eq. 28) is numerically unstable at low temperatures and strong couplings. That is, the product has a very high ratio of largest to smallest eigenvalue. Special "stabilization" is required to do the matrix manipulations. While these add to the complexity of the code, they however have no content in the sense that all the above equations are valid, it is just a question of how best to multiply matrices on a machine of finite precision.

(3.) The determinants of the matrices can go negative. This is called the "fermion sign problem." The sign problem does not occur for certain special cases. For example, if U is negative (the "attractive" Hubbard model), the individual determinants can go negative, but the matrices are always equal and hence the determinant appears as a perfect square. This is a consequence of the fact that the appropriate Hubbard–Stratonovich transformation

couples S to the charge $n_\uparrow + n_\downarrow$ as opposed to the spin as given in Eq. 25 for the repulsive model. If U is positive but the chemical potential $\mu = U/2$ ("half–filling") one is also okay. The matrices are not identical in this case, but the determinants are nevertheless related by a positive factor, that is, they again have the same sign, so their product is always positive. Some types of randomness are also acceptable. It is okay for the hoppings t and interactions U to depend on the link or site. These statements are demonstrated by various particle–hole transformations on the Hamiltonian.
(4.) Alternate Hubbard–Stratonovich transformations are possible. One can couple more symmetrically to the spin, that is not single out the z component Or, one can couple to pair creation operators. So far, all such alternatives give a worse sign problem than the transformation Eq. 25. These more complicated transformations are needed to do 'Hund's rule terms' in multi-orbital Hubbard models.
(5.) Very similar "ground state" determinant simulations exist which work at $T = 0$ and in the canonical ensemble.

What Determinant QMC Simulations Can Do

The state of the art of determinant QMC simulations, in the absence of a sign problem, are studies of several hundred electrons down to temperatures of $\beta t = 10 - 20$. In terms of temperature and bandwidth, this means T of roughly $1/100$ of the bandwidth $W = 8t$ of the 2-d Hubbard model. This is plenty cold enough to see well developed magnetic correlations. For typical parameters, $t = 1, U = 4$ one chooses $\Delta\tau = 1/8$ so these beta values correspond to roughly $L = 100$, and the simulation involves approximately 10^4 Hubbard–Stratonovich variables.

In cases where one has a sign problem, βt is limited to 4–5. This is, unfortunately, not low enough in temperature to make conclusive statements about certain important problems, perhaps most prominently the question of the existence of long range $d-$wave superconducting correlations in the Hubbard model away from half-filling.

Some Results

The evolution of the local moment (Eq. 12) at half-filling as the temperature is decreased is shown in Fig. 1 on a 6x6 lattice for different interaction strengths U. We see the local moment begin to develop from its uncorrelated value $\frac{1}{2}$ at a temperature set by U, and then saturate at low T. The local moment does not reach 1 at $T = 0$ because significant quantum fluctuations allow doubly occupied and empty sites to occur even in the ground state. However, as U increases, these fluctuations are suppressed and the moment becomes better and better formed. The local moment also makes a further small adjustment at low T, which is due to the onset of long range magnetic order.

From the energy we can get the specific heat (Fig. 2). It shows an interesting two peak strudture. The high temperature peak is associated with the formation of local moments, and the low temperature peak with their ordering. The Hubbard model maps onto the Heisenberg model at large U. This connection is emphasized in Fig. 2 which shows that the

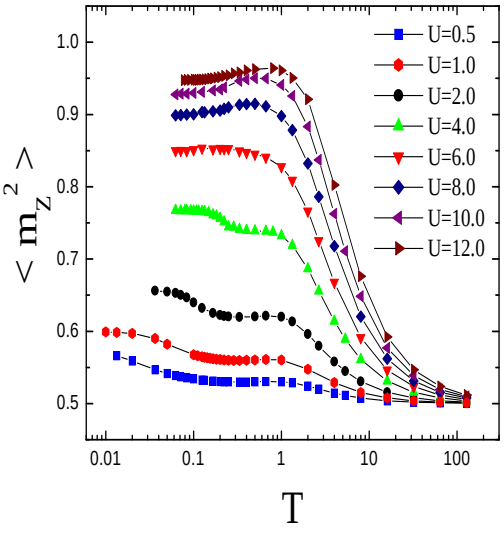


FIG. 1: The local moment $\langle m_z^2 \rangle$ as a function of temperature for different interaction strengths U and lattice size 6x6. The lattice is half-filled.

low temperature peak in the specific heat of the Hubbard model can be mapped onto that of the Heisenberg model with $J = 4t^2/U$.

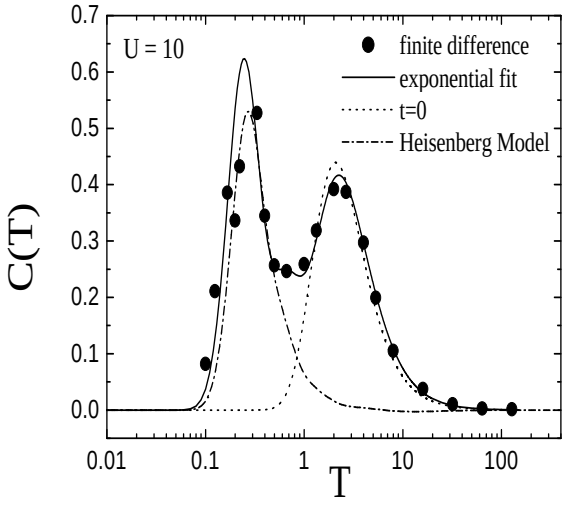
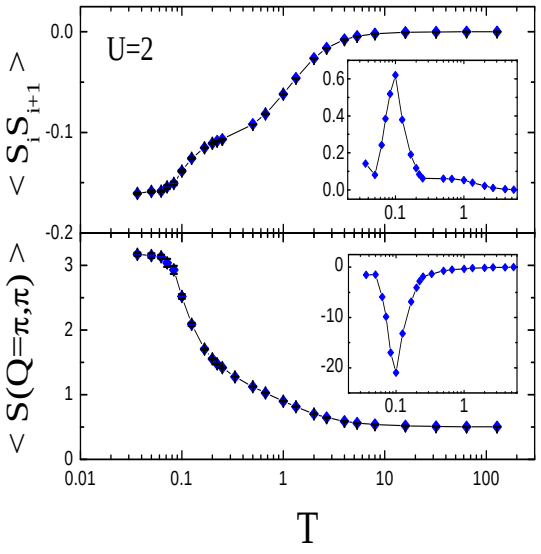


FIG. 2: The specific heat of the Hubbard model for $U = 10t$. There is a high temperature peak which is fit well by considering a single site Hubbard model ($t = 0$) and a low temperature peak which agrees well with the Heisenberg model with $J = 4t^2/U = 0.4$.

The near-neighbor spin correlation are shown in Fig. 3. The magnetic structure factor $S(\pi, \pi) = \frac{1}{N} \sum_{ij} \langle S_{z,i} S_{z,j} \rangle$ sums these correlations over the whole lattice. It is found that

$S(\pi, \pi)$ grows linearly with N at low T, indicating that the correlations extend over the whole lattice.



The near neighbor spin correlations and magnetic structure factor of the half-filled Hubbard model at $U = 2t$.

FIG. 3:

Finally, in Fig. 4 we show the density of states at $\omega = 0$ for the half-filled Hubbard model at different values of U. The suppression of $N(\omega = 0)$ at low T and large U is a signature of the presence of an insulating gap caused by the on-site repulsion.

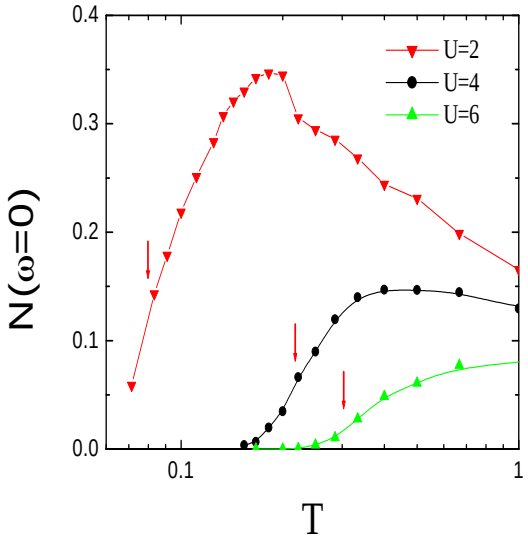


FIG. 4: The density of states at $N(\omega = 0)$. As T is lowered, a Mott-Hubbard gap opens up. The half-filled Hubbard model is insulating.

Conclusions

Determinant QMC is a powerful method for simulating interacting electron Hamiltonians in more than one dimension. One can easily study problems with several hundred particles, an order of magnitude greater than with exact diagonalization, and often large enough to make compelling finite size scaling analysis. The sign problem is a very significant limitation, however. For the repulsive Hubbard model, one can go to temperatures on the order of $W/30$ where W is the bandwidth. For special cases like the attractive Hubbard model or the repulsive model at half-filling, there is no sign problem, and the ground state properties can be obtained.

Algorithm development in determinant QMC currently focusses on applications to DMFT, where the Hubbard-Stratonovich field is allowed to fluctuate only in imaginary time. A number of questions are being actively explored in this field: How does one incorporate more complex (e.g. Hund's rules) interactions into simulation which include multiple orbitals? Can one re-introduce some degree of spatial fluctuations?