Abstract

We present a pedagogical discussion of a quantum Monte Carlo method for correlated lattice systems in the infinite-dimensional limit. We discuss the underlying theory, Metzner and Vollhardt’s Dynamical Mean field theory, which becomes exact in infinite dimensions. Also included is the formalism necessary to describe lattice properties using only the local information which can be gleaned from the QMC procedure. We then derive the QMC algorithm using a compact Grassmann notation, and apply this algorithm to solve the infinite dimensional Hubbard model. We show that it retains many of the transport anomalies and features of the phase diagram expected of the finite-dimensional model, and seen in the cuprate high-temperature superconductors.
1 Introduction

Some of the most exotic properties of materials, including high-temperature superconductivity, magnetism, and heavy Fermion and non-Fermi liquid behaviors, are due to strong electronic correlations. The materials which display these properties are characterized by either narrow electronic bands or compact orbitals with large angular momentum in the valence shell. In either case, the potential energy associated with some of these electronic degrees of freedom is of similar magnitude or larger than their electronic kinetic energy (bandwidth). Thus, these materials cannot be studied by perturbing around either the atomic or free band limits, making the \textit{ab initio} study of these complicated systems difficult. Thus, we resort to the construction of simplified models to study these systems.

For example, the Hubbard model\cite{1} is the simplest model of a correlated electronic lattice system. Both it and the $t - J$ model are thought to at least qualitatively describe some of the properties of transition metal oxides, and possibly high temperature superconductors\cite{2}. The Periodic Anderson model along with various Kondo lattice models have been proposed to describe both the Actinide and Lanthanide Heavy Fermion systems and the Anderson insulators. The Holstein model incorporates the essential physics of strongly interacting electrons and phonons. All of these model
Hamiltonians contain at least two major ingredients: a local interaction term and a non-local hopping term. For example, the Hubbard model Hamiltonian is

$$H = -\frac{t^*}{2\sqrt{d}} \sum_{\langle j,k \rangle} (c_{j\sigma}^\dagger c_{k\sigma} + c_{k\sigma}^\dagger c_{j\sigma}) + \sum_j \epsilon (n_{j\uparrow} + n_{j\downarrow}) + U (n_{j\uparrow} - 1/2) (n_{j\downarrow} - 1/2),$$  \hspace{1cm} (1)

where $c_{j\sigma}^\dagger$ ($c_{j\sigma}$) creates (destroys) an electron at site $j$ with spin $\sigma$, $n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma}$, and $t^* = 1$ sets our unit of energy.

However, except for special limits, even such simplified models like (1) cannot be solved exactly. For example, for the Hubbard model, no exact solutions exist except in one dimension, where the knowledge is in fact rather complete [3]. The Periodic Anderson model is only solvable in the limit where the orbital degeneracy diverges [4], and the Holstein model is only solvable in the Eliashberg-Migdal limit where vertex corrections may be neglected. Clearly a new approach to these models is needed if nontrivial exact solutions are desired.

Recently, Metzner and Vollhardt suggested such a new approach [5, 6, 7] based on an expansion in $1/d$ about the point $d = \infty$ to study these strongly correlated lattice models. The resulting formalism neglects dynamical intersite correlations while retaining the important local dynamical correlations. The resulting formalism is called \textit{Dynamical Mean Field Theory} since it may be employed in any dimension. In this article, we discuss a quantum Monte Carlo (QMC) algorithm used to numerically solve model systems in the infinite dimensional limit. In each section, we will demonstrate these methods using the Hubbard model (Eq. 1) on a hypercubic lattice; however, these techniques may be readily applied to each of the model Hamiltonians mentioned above. This article is organized as follows: In the next section, Sec. 2, we will discuss the dynamical mean field formalism and the formalism needed to calculate non-local quantities. The QMC algorithm and the measurement of local quantities will be discussed in Sec. 3. In Sec. 4, we will discuss the application of this method to the Hubbard model as an example.

\section{Formalism}

\subsection{The Infinite Dimensional Limit}

The correlated lattice problem simplifies greatly in the infinite-dimensional limit [5]. Models with variants of hypercubic lattices obtain a simple Gaussian bare density of electronic states (DOS), the self energy and all of the irreducible vertex functions become momentum independent, dynamical intersite correlations vanish and transitions driven exclusively by non-local correlations (i.e., with no relevant local effects such as screening) become mean-field transitions, and the problem may be mapped onto a corresponding self-consistently embedded impurity problem.

On a hypercubic lattice, each site has $2d$ nearest neighbors, $2d(d - 1)$ next nearest neighbors, etc. If $d$ is large, for any site the fluctuations of any one of its nearest
neighbors produces an effect of order $1/d$ and may be neglected. Thus, the hypercubic lattice is a natural venue for developing a mean-field theory. The infinite-dimensional Brillouin zone for the hypercubic lattice retains the hypercubic geometry. Only the points at the zone center and corner are unique. The degeneracy of all other points diverges. The points are described by

$$x(q) = \frac{1}{d} \sum_{l=1}^{d} \cos(k_l),$$

(2)

which defines a set of the equivalent points in the infinite-dimensional Brillouin zone.

The origin of the Gaussian bare density of states can be understood from arguments based on the central limit theorem since each direction in the infinite-dimensional Brillouin zone contributes independently to the density of states. The mean square energy contributed by each direction is $2t^2$. Thus, with $d$ independent directions, the bare density of states is a Gaussian

$$\rho^0(\epsilon) = \sqrt{\frac{1}{4t^2d\pi}} \exp(-\epsilon^2/4t^2d)$$

(3)

with width $2\sqrt{dt^2}$. This must remain finite as $d \to \infty$ in order for the physics of the free-electron system to remain sensible (i.e. for the bare electron energy to remain finite). This can only happen if $dt^2 = \text{constant}$ as $d \to \infty$. Typically, one uses this to define a unit of energy $t^* = 2t\sqrt{d} = 1$. It is interesting to note that the constancy of $t^*$ as $d \to \infty$ also insures that the magnetic properties of Hubbard-like models will remain interesting. In a mean-field based theory we expect that transition temperature to go roughly as the net magnetic exchange between any site and its set of $2d$ nearest neighbors, $2dJ \sim -4dt^2/U$. This remains finite as $d \to \infty$ and hence, so does the transition temperature.

**Single-Particle Self Energy and the Mapping to the Impurity**

The locality of the self energy (i.e., its momentum independence) can be understood from simple diagrammatic arguments. The single-particle Green’s functions $G(R, i\omega_n) \sim t^R$ to leading order in the hybridization $t$, thus they fall off very quickly with distance in this limit, $G(R, i\omega_n) \sim d^{-R/2}$, so that nonlocal diagrams in the irreducible self energy (and two-particle irreducible vertices) may be neglected. For example, consider the second order Hubbard self energy diagram shown in Fig. 1. If sites $i$ and $j$ are nearest neighbors, then this contribution to the self energy scales like $t^3 \sim 1/d^{5/2}$ which vanishes in the infinite-dimensional limit. In fact, the contributions from the next nearest neighbor shell, etc. also vanish. The only contribution which survives in the infinite-dimensional limit is the local one for which $i = j$.

Thus, the self energy for the single-particle Green’s function and the irreducible vertex functions have no momentum dependence and are functionals of the local
Figure 1: Second order contribution to the self energy of the Hubbard model. Here, the solid lines represent the undressed ($U = 0$) electron propagators $G^0_{ij}(i\omega_n)$, and the dashed lines represent the intrasite interaction $U$. If sites $i$ and $j$ are nearest neighbors, then this diagram scales like $t^3 \sim 1/d^{3/2}$ which vanishes when $d \to \infty$. Only the local contribution $i = j$ survives.

Figure 2: First few diagrams for the self energy of the infinite-dimensional Hubbard model. Note that this is the same diagrammatic series as that for the self energy of the Anderson impurity model, but to avoid overcounting the local self energy (c.f. the third order in $U$ diagram) it is necessary to subtract the local self energy to define the local propagator $G$ represented by the solid line, $G(i\omega_n)^{-1} = G(i\omega_n)^{-1} + \Sigma(i\omega_n)$, where $G(i\omega_n) = G(R = 0, i\omega_n)$

Green's function [5, 8] and the interaction. The first few terms of the diagrammatic series for the Hubbard model self energy is shown in Fig. 2. This is the same diagrammatic series as that for the self energy of the Anderson impurity model; however, in order to not overcount the local self energy (c.f. the third order in $U$ diagram) it is necessary to subtract the local self energy from the local propagator $G$ which defines the solid line. $G(i\omega_n)^{-1} = G(i\omega_n)^{-1} + \Sigma(i\omega_n)$, where $G(i\omega_n) = G(R = 0, i\omega_n)$ is the full local Green’s function. Thus, the self energy of the infinite-dimensional Hubbard model is a functional of the site-excluded Green’s function and the local interaction $\Sigma(G, U)$; it has the same diagrammatic expansion as an Anderson impurity with local interaction $U$ and local (host) Green’s function $G(i\omega_n)$, given by $G(i\omega_n)^{-1} = G(i\omega_n)^{-1} + \Sigma(i\omega_n)$.

We may construct an algorithm, sketched in Fig. 3, to solve the infinite-dimensional Hubbard model (and most other infinite-dimensional lattice problems) by [9, 10, 11]
(i) making an initial guess for the self energy from perturbation theory, (ii) calculating the corresponding local Green’s function

\[ G(i\omega_n) = \int d\epsilon \frac{\rho^0(\epsilon)}{i\omega_n - \epsilon - \Sigma(i\omega_n)} = -i\sqrt{\pi} w(i\omega_n - \epsilon - \Sigma(i\omega_n)) \]  

(4)

where \( w(z) \) is the Faddeev function, (iii) calculating the host Green’s function \( G(i\omega_n)^{-1} = G(i\omega_n)^{-1} + \Sigma(i\omega_n) \), (iv) using QMC (or NRG, or perturbation theory like the non-crossing approximation, etc.) to obtain the \( G(i\omega_n) \) for the corresponding impurity problem, (v) using this and the initial Green’s function \( G(i\omega_n) \) to construct a new self energy \( \Sigma(i\omega_n) = G(i\omega_n)^{-1} - G(i\omega_n)^{-1} \), and repeating this entire process until convergence is reached. Finally, an additional QMC step is required to measure a variety of local one and two-particle properties of the model. Local dynamical quantities can be calculated by analytically continuing the corresponding local Green’s functions using the Maximum Entropy Method[12, 13], which will be discussed in Chapter X.

Figure 3: Flowchart for the \( d = \infty \) algorithm. Starting from the host Green’s function \( G(i\omega_n) \), the self energy is calculated with the QMC algorithm of Hirsch and Fye[28, 29]. The local one and two-particle Green’s functions (\( G(\tau) \) and \( \chi(\tau) \)) may be analytically continued to real frequencies using the maximum entropy method (MEM).

2.2 Physical Quantities in Infinite Dimensions

The calculation of non-local momentum-dependent, or lattice, quantities requires additional formalism, which will be discussed in this section. Many experimentally relevant quantities can be studied with this QMC process and a reasonable amount of computational effort. For example, the equilibrium transport and one-particle properties may be studied in both real and imaginary frequency, and many two-particle properties may also be calculated. However, most of these quantities cannot be directly measured in the QMC process; rather, we measure some local quantities from which we extract irreducible diagrammatic functions which are used to construct the quantity of interest.
**Single-Particle Properties**

For example, the single-particle self energy $\Sigma(z)$, allows us to calculate all of the other single-particle properties of the system. As discussed in Sec. 2.1, $\Sigma(i\omega_n)$ is a by product of the self-consistent procedure shown in Fig. 3; however, the calculation of $\Sigma(\omega)$, evaluated at real frequencies $\omega$, requires numerical analytic continuation, discussed in Chapter X. For a variety of reasons, we find it more efficient to analytically continue the local Green’s function $G(\omega)$ and then extract the self energy by inverting

$$G(\omega) = -i\sqrt{\pi}w (\omega - \epsilon - \Sigma(\omega)) .$$

(5)

In most cases, perturbation theory[14] was used to provide an initial, high-temperature, default model for this procedure. $G(\omega)$ at lower temperatures are then produced with the “annealing procedure”[12]. We then solve Eq. 5 for $\Sigma(\omega)$ using a complex root finder.

**Optical and Transport Properties**

Knowledge of $\Sigma(\omega)$ is all that is needed to calculate the electrical conductivity, and the optical conductivity, and to estimate the thermopower, thermal conductivity, and the Hall coefficient[15]. For example, an exact expression for the conductivity may be calculated following the discussion of Ref. [15]. Figure 4 shows the leading diagrams in the expansion of the conductivity. The particle-hole vertex appearing in

![Figure 4: Diagrammatic representation of the first two contributions to the conductivity. The second diagram contains a full particle-hole vertex insertion. The latter is momentum independent, i.e., the $k$-sums on both sides can be performed independently. Since the current vertex and the single-particle Green functions are of different parity (with respect to their $k$-dependence) the second and all higher-order diagrams identically vanish.](image)

the second and all higher-order diagrams is momentum independent since it can be written as a functional derivative of the momentum-independent self energy. This means that the $k$-sums on the left and right end of all diagrams, except for the simple bubble, may be performed independently. Since the current operator contains the $k$-gradient of the kinetic energy, and the Green functions are $k$-dependent only through
\( \epsilon_k \), these sums identically vanish. Thus the conductivity is given by the simple bubble only \([16, 17, 18]\). The evaluation of the bubble leads to

\[
\sigma_{xx}(\omega) = \frac{\pi e^2}{2\hbar a} \int_{-\infty}^{\infty} d\epsilon \frac{f(\epsilon) - f(\epsilon + \omega)}{\omega} \frac{1}{N} \sum_{k\sigma} \left( \frac{\partial \epsilon_k}{\partial k_x} \right)^2 A(\epsilon_k, \epsilon) A(\epsilon_k, \epsilon + \omega) ,
\]

which reduces to

\[
\sigma = \frac{e^2 \pi}{2\hbar a} \int_{-\infty}^{\infty} d\epsilon \left( \frac{\partial f(\epsilon)}{\partial \epsilon} \right) \frac{1}{N} \sum_{k\sigma} \left( \frac{\partial \epsilon_k}{\partial k_x} \right)^2 [A(\epsilon_k, \epsilon)]^2 ,
\]

for the dc conductivity, where \( a \) is the lattice constant, \( A(\epsilon_k, \epsilon) = -\frac{1}{\pi} \text{Im} [G(\epsilon_k, \omega)] \), and \( f(\epsilon) = 1/[1 + \exp \beta \epsilon] \) is Fermi’s function. With \( h/e^2 \approx 2.6 \times 10^4 \Omega \) the constants in front of Eq. (7) can be evaluated to yield \( \sigma_0 \approx 10^{-3} \ldots 10^{-2} [(\mu \Omega \text{cm})^{-1}] \).

The Drude weight \( D \), may be determined by extrapolation of the Matsubara-frequency current-current correlation function using the method proposed by Scalapino et al.\([19]\). This method sets a criterion to determine if the ground state of a system is a metal, insulator, or superconductor, by determining the asymptotic form of the current-current susceptibility in the x-direction, \( \Lambda_{xx}(\mathbf{q}, i\nu_n) \) where \( \nu_n = 2n\pi T \). Specifically, the Drude weight, \( D \), is given by

\[
D = \pi \lim_{T \to 0} \left[ \langle -T_x \rangle e^2 - \Lambda_{xx}(\mathbf{q} = 0, 2\pi i T) \right] .
\]

Here, \( \langle -T_x \rangle \) is the average kinetic energy per site.

Comparison of Eq. 6 with the standard expressions for transport coefficients \([20]\) in the relaxation-time approximation, shows that a variety of other transport coefficients may be calculated if one identifies

\[
\tau_{xx}(\epsilon) = \frac{1}{N} \sum_{k\sigma} \left( \frac{\partial \epsilon_k}{\partial k_x} \right)^2 [A(\epsilon_k, \epsilon)]^2
\]

as the transport relaxation time. For example, the electronic contribution to the thermopower becomes \([18, 20]\]

\[
S = -\frac{k_B}{|e|} \beta \frac{L_{12}}{L_{11}} , \quad \frac{k_B}{|e|} \approx 86 [\mu \text{V/K}] ,
\]

where \( L_{jk} \) are the standard transport integrals

\[
L_{jk} = \int_{-\infty}^{\infty} d\epsilon \left( -\frac{\partial f(\epsilon)}{\partial \epsilon} \right) \tau^j(\epsilon) \epsilon^{k-1} .
\]

It is known from studies of heavy fermion systems that the relaxation-time approximation is sufficient to understand most zero-field properties. The Hall coefficient, however, is more sensitive to the approximations involved: Within the standard relaxation-time approximation the Hall coefficient satisfies

\[
R_H = \frac{1}{-\epsilon} \frac{L_{11}}{L_{21}} .
\]
Note that both $L_{11}$ and $L_{21}$ are positive, implying that the Hall-coefficient is always negative and that the transport is electron-like. On the other hand, experiments show that $R_H$ can change sign in intermediate or low temperature regions, and that the Hall coefficient is usually positive with an anomalous temperature dependence. However, a more refined treatment of the field-dependent conductivity can be performed [21]. The result is

$$\sigma_{xy}^H = \frac{2\pi^2 |e|^3 a B}{3\hbar^2} \int_{-\infty}^{\infty} d\omega \left( \frac{\partial f(\omega)}{\partial \omega} \right) \frac{1}{N} \sum_{k\sigma} \left( \frac{\partial \epsilon_k}{\partial k_x} \right)^2 \frac{\partial^2 \epsilon_k}{\partial k_y^2} [A(\epsilon_k, \omega)]^3, \quad (13)$$

for the Hall conductivity. Here, $B$ is the external magnetic field which points in the $z$-direction. The constants in Eq. (13) can be rearranged according to $|e|^3 a B/\hbar^2 = \sigma_0 |e| a^2 B/\hbar$ and $|e| a^2 B/\hbar \approx 10^{-5} B \left[ \frac{1}{T} \right]$. Inserting the values for $\sigma_0$, we obtain $R_H = \sigma_{xy}/\sigma_{xx} \approx 10^{-8} \ldots 10^{-9} B \left[ m^3 / cT \right]$ as the unit for the Hall coefficient.

In the limit of large $d$, and for a simple hypercubic lattice, the $k$-sums in Eqs. (9) and (13) can be further simplified to yield

$$\frac{1}{N} \sum_{k\sigma} \left( \frac{\partial \epsilon_k}{\partial k_x} \right)^2 K(\epsilon_k) = \frac{2}{d} \int_{-\infty}^{\infty} d\epsilon \rho_0(\epsilon) K(\epsilon), \quad (14)$$

and

$$\frac{1}{N} \sum_{k\sigma} \left( \frac{\partial \epsilon_k}{\partial k_x} \right)^2 \frac{\partial^2 \epsilon_k}{\partial k_y^2} K(\epsilon_k) = -\frac{1}{2d^2} \int_{-\infty}^{\infty} d\epsilon \rho_0(\epsilon) \epsilon K(\epsilon), \quad (15)$$

with $K(\epsilon_k)$ an arbitrary function depending on $k$ through $\epsilon_k$ only.

Examination of Eqs. 6,13–15 shows that the electronic conductivity is a $1/d$ effect and that the Hall effect enters to order $1/d^2$. In our calculations we determine lowest-order quantities and calculate the coefficient of the $1/d$ term for $\sigma_{xx}$ and the coefficient of the $1/d^2$ term for $\sigma_{xy}$ (i.e., $\sigma_{xx} \rightarrow d \cdot \sigma_{xx}$ and $\sigma_{xy} \rightarrow d^2 \cdot \sigma_{xy}$). Note, however, that $R_H = \sigma_{xy}/\sigma_{xx}^2$ enters to zeroth order and requires no rescaling!

**Static Susceptibilities**

Both the local and momentum-dependent two-particle Green’s functions may also be calculated with this approach at any value of $x(q)$. Since the self-energy is local, so are the irreducible vertex functions since they may be obtained from functional derivatives of the self energy (i.e., $\Gamma_{\sigma,\sigma'} = \delta \Sigma_\sigma / \delta G_{\sigma'}$). Thus, the two-particle Dyson equations for the local and lattice two-particle propagators share the same irreducible vertex function.

For example, the two-particle Dyson’s equation for the lattice and local particle-particle opposite spin propagators are shown in Fig. 5. The corresponding equations are

$$\chi_q = \chi_{q0} + \chi_{q0} \Gamma \chi_q \quad (16)$$
\[ \chi = \chi_0 + \chi_0 \Gamma \chi. \]  

(17)

Here, \( \chi_{q0} \) is the lattice momentum dependent two-particle propagator without vertex corrections (i.e., the simplest bubble diagram involving the fully dressed single-particle propagator). It may be calculated with the methods developed by Müller-Hartmann[6, 22].

\[
\chi_{q0}(i\omega_n, i\omega_m) = \frac{\delta_{nm}}{N} \sum_k G(\epsilon_k, i\omega_n)G(\epsilon_{k+q}, i\omega_n) = \delta_{nm} \int \int d\epsilon_1 d\epsilon_2 \rho(\epsilon_1, \epsilon_2, q)G(\epsilon_1, i\omega_n)G(\epsilon_2, i\omega_n). \tag{18}
\]

In infinite dimensions, the two-particle density of states becomes

\[
\rho(\epsilon_1, \epsilon_2, q) = \frac{1}{N} \sum_k \delta(\epsilon_1 - \epsilon_k)\delta(\epsilon_2 - \epsilon_{k+q}) = \frac{1}{\pi \sqrt{1 - x(q)^2}} \exp \left[ -\frac{1}{2} \left( \frac{(\epsilon_1 - \epsilon_2)^2}{1 - x(q)} + \frac{(\epsilon_1 + \epsilon_2)^2}{1 + x(q)} \right) \right]. \tag{19}
\]

Using the self energy calculated in the QMC procedure, \( \chi_{q0} \) may be calculated at any value of \( x(q) \). The local two-particle Green’s functions may similarly be calculated. For example, \( \chi_0 \) is the local undressed two-particle propagator, which may be constructed from the local single-particle propagator \( \chi_0 = G^2(i\omega_n) \), and \( \chi \) is measured in the Monte Carlo process[10], as described in Sec. 3.2. Thus, we can solve Eq. 17 for the corresponding vertex function matrix \( \Gamma \) used in Eq. 16 to calculate \( \chi_q \). Quite generally, the two-particle propagators with the same symmetry as the lattice, and that involve no net frequency transfer, \( \chi_q(i\omega_n, i\omega_m) \) are related to the corresponding local propagator \( \chi(i\omega_n, i\omega_m) \) by the following matrix form

\[
\chi_q^{-1} = \chi_{q0}^{-1} + \chi^{-1} - \chi_0^{-1}. \tag{20}
\]

In fact, two-particle propagators which probe transitions to ordered states with symmetry orthogonal to the lattice symmetry, such as that for superconductivity with lower symmetry than s-wave, generally have no vertex corrections due to the lack of momentum dependence of the vertex functions[23]. Thus, Eq. 20 holds for all cases of interest, and the corresponding static susceptibility is calculated by summing over Matsubara frequencies

\[
\chi_q(T) = T \sum_{n,m} \chi_q(i\omega_n, i\omega_m). \tag{21}
\]

This formalism may easily be modified to construct charge and even-frequency superconducting bulk susceptibilities.

However, odd-frequency superconductivity[24] is also possible in strongly correlated infinite-dimensional systems. In systems with a strong local repulsive interaction, a transition to an on-site s-wave state (or any other state within the same
subgroup) is unlikely. Rather, to circumvent the strong local correlation, the superconductivity is favored in channels with either a spatial or temporal gap. As discussed above, in the infinite-dimensional limit, the former lacks vertex corrections which could drive a transition, leaving superconductivity in a state with a temporal gap, or odd-frequency superconductivity, the only likely candidate.

To explore this possibility, we use the methods described above to extract superconducting vertex function $\Gamma_s$ from the local pair-field susceptibility matrix, and construct the undressed lattice pair-field susceptibility $P_{q0}(i\omega_n, i\omega_m)$. We may then write down the two-particle Dyson’s equations for the fully-dressed pair-field susceptibility $P_q(i\omega_n, i\omega_m)$ matrix

$$P_q = P_{q0} + P_{q0}\Gamma_sP_{q0} + P_{q0}\Gamma_sP_{q0}\Gamma_sP_{q0} + \cdots .$$  (22)

This equation may be rewritten as

$$P_q = \sqrt{P_{q0}}\left[I - \sqrt{P_{q0}\Gamma_s}\sqrt{P_{q0}}\right]^{-1}\sqrt{P_{q0}} .$$  (23)

The nature of the transition is dictated by the dominant eigenvalue and eigenvector of the pairing matrix[25]

$$M_q = \sqrt{P_{q0}\Gamma_s}\sqrt{P_{q0}} .$$  (24)

For example, the system will undergo a conventional second-order transition when the dominant eigenvalue of $M_q$ first increases to one. However, if the eigenvector corresponding to the dominant eigenvalue is odd, then its effect will vanish when we sum $M_q$ over all Matsubara frequencies to form the static pair-field susceptibility. In order to project out the odd-frequency pair-field susceptibility, we must use an odd in frequency form factor $f(i\omega_n) = -f(-i\omega_n)$.

$$P_{q0}(T) = T\sum_{n,m} \phi(i\omega_n)P_q(i\omega_n, i\omega_m)\phi(i\omega_m)$$

(25)
\( \phi \) may be determined by analytic arguments, or it may even be the dominant odd eigenvector of \( \mathbf{M}_q \) divided by \( \sqrt{\mathbf{P}_{q0}} \). The only restriction is that it should not be orthogonal to the leading form of the order parameter at the transition.

Another important probe of correlated electronic systems involves nuclear magnetic resonance (NMR). The spin-lattice relaxation time \( T_1 \) characterizes the time needed to align the nuclear spins along the direction of the field. The local NMR-relaxation rate satisfies

\[
\frac{1}{T_1} = T \lim_{\omega \to 0} \text{Im} \frac{\chi(\omega)}{\omega},
\]

where \( \chi(\omega) \) is the local dynamic spin susceptibility. Similarly, the spin-echo decay rate (or transverse nuclear relaxation rate) \( T_{2G} \) probes the spin dynamics, and may also be calculated in the infinite-dimensional limit\[15\]. \( T_{2G} \) satisfies a more complicated relation\[26, 27\]

\[
\left[ \frac{1}{T_{2G}} \right]^2 = C \left[ \sum_k F(k)^4 \chi(x(k))^2 - \left\{ \sum_k F(k)^2 \chi(x(k)) \right\}^2 \right],
\]

with \( \chi(x(k)) \) the static momentum-dependent spin susceptibility, \( C \) an overall normalization factor, and \( F(k) \) the relevant form factor. The form factor involves the local site and the nearest-neighbor shell, and assumes the form

\[
F(k) = 1 + \gamma \frac{2t}{U} e^{i k \cdot \mathbf{r_k}}.
\]

in infinite dimensions. Here, \( \gamma \) is a constant of order 1. The static susceptibility with \( x = 0 \) corresponds to the local susceptibility. The integrals over the form factors can be performed, to yield

\[
\left[ \frac{1}{T_{2G}} \right]^2 = C \frac{d}{d} \left[ 2\gamma^2 \chi^2(x = 0) - \frac{1}{2} \left| \frac{d \chi(x)}{dx} \right|_{x=0}^2 \right].
\]

The inverse spin-echo decay rate is a \( 1/\sqrt{d} \) effect in infinite dimensions, and it is effectively proportional to the local susceptibility, since the derivative of the momentum-dependent susceptibility with respect to \( x \) is an order of magnitude smaller than the susceptibility itself in the region of interest (see Fig. 8). In fact, we neglect the derivative term when evaluating \( T_{2G} [T_{2G} \propto 1/\chi(x = 0)] \).

### 3 The QMC Algorithm

In the Sec. 2, we outlined a technique to solve the infinite-dimensional lattice problem if we can solve the corresponding impurity problem. We use the algorithms of Hirsch and Fye to solve the impurity problems. In this section we will derive the Hirsch-Fye Anderson impurity algorithm. We will then discuss the modifications
necessary to adapt this algorithm to simulate infinite-dimensional lattice models, and discuss how various measurements are made. Fye and Hirsch also developed algorithms which can be used to simulate spin lattice problems such as the Kondo lattice problem (multiple channels and orbital degeneracy can also be treated). We will not provide a detailed derivation of these algorithms here; rather, we refer the reader to [28, 29].

3.1 The Hirsch-Fye Algorithm

We will derive the Hirsch-Fye Anderson impurity algorithm[28] using Grassmann algebra. We begin by splitting the Single Impurity Anderson Model Hamiltonian, into bare and interacting parts, \( H_{SIAM} = H_0 + H_I \), where

\[
H_0 = \sum_{k,\sigma} (\epsilon_c + \epsilon_k) c^\dagger_{k,\sigma} c_{k,\sigma} + V \sum_{k,\sigma} (f^\dagger_{\sigma} c_{k,\sigma} + c^\dagger_{k,\sigma} f_{\sigma}) + \epsilon(n_\uparrow + n_\downarrow)
\]  

(30)

and

\[
H_I = U(n_{f\uparrow} - 1/2)(n_{f\downarrow} - 1/2).
\]  

(31)

To obtain the Trotter-Suzuki decomposition for the partition function [30] we divide the interval \([0, \beta]\) into \(L\) sufficiently small subintervals such that \(\Delta \tau^2 [H_0, H_I]\) may be neglected. This leads to

\[
Z = Tr e^{-\beta H} = Tr \prod_{l=1}^{L} e^{-\Delta \tau H} \approx Tr \prod_{l=1}^{L} e^{-\Delta \tau H_0} e^{-\Delta \tau H_I}.
\]  

(32)

The interacting part of the Hamiltonian may be further decoupled by mapping it to an auxiliary Ising field via a discrete Hirsch-Hubbard-Stratonovich[31] transformation,

\[
e^{-\Delta \tau H_I} = e^{-\Delta \tau U(n_{f\uparrow} - 1/2)(n_{f\downarrow} - 1/2)} = 1/2 e^{-\Delta \tau U/4} \sum_{s=\pm 1} e^{\alpha s (n_{f\uparrow} - n_{f\downarrow})}
\]  

(33)

where \(\cosh(\alpha) = e^{\Delta \tau U/2}\). One may cast Eq.32 into functional-integral form by using Grassmann variables for Fermions. If we integrate out the host Fermionic degrees of freedom \(\{c_{k,\sigma}\}\), then we end up with

\[
S_{eff} = (\Delta \tau V)^2 \sum_{l,l',\sigma} f^*_{\sigma,l} G_0(l,l') f_{\sigma,l'} + S_{int},
\]  

(34)

where \(f_{\sigma,l}\) and \(f^*_{\sigma,l}\) are Grassmann variables representing the impurity Fermionic degrees of freedom.

\[
S_{int} = \sum_{l,\sigma} -f^*_{\sigma,l} (f_{\sigma,l} - f_{\sigma,l-1}) + \Delta \tau f^*_{\sigma,l} (\epsilon_f + U/2 + \frac{\alpha}{\Delta \tau} s_{l,\sigma}) f_{\sigma,l-1}
\]  

(35)

and

\[
G_0^{-1}(l,l') = \frac{1}{N} \sum_{k} \delta_{l,l'} - \delta_{l-1,l'} (1 - \Delta \tau \epsilon_k).
\]  

(36)
At this point the correspondence of the single-impurity model and the infinite-dimensional Hubbard model is clear. In both, $G_0$ contains the information about the host into which the impurity is embedded. The difference is that $G_0$ is given by Eq. 36 for the impurity model, but must be determined self-consistently for the lattice model (c.f. Fig. 3).

We will now proceed to derive the Monte Carlo algorithm\[28\] sufficient for either the impurity or the infinite-dimensional lattice problem. By integrating over $f_{\sigma l}$ we can write down the partition function (neglecting a numerical prefactor), as

$$Z = \sum_{\{s_l\}} \det(G_{\{s_l\}}^{-1}) \det(G_{\{s_l\}}^{-1})$$

where

$$G_{\sigma,\{s_l\}}^{-1}(l, l') = \delta_{l,l'} - \delta_{l-1,l'} (1 - \Delta \tau \epsilon_f + \alpha s_l \sigma) - \Delta \tau^2 V^2 G_0(l, l')$$

and we sum over all configurations of Hubbard-Stratonovich field $\{s_l\}$. If we re-exponentiate the above formula by defining $V_{\sigma,\{s_l\}}(l) \equiv \Delta \tau (\epsilon_f + \alpha s_l \sigma / \Delta \tau)$, we can write it in a simple notation as

$$G_{\sigma}^{-1} = 1 + T e^{V_\sigma} + \Delta \tau^2 V^2 G_0,$$

where $T$ is $\delta_{l-1,l}$ and $V_\sigma \equiv V_{\sigma,\{s_l\}}(l)$ for one special configuration. For another field configuration the only difference comes from $V_\sigma$ such that $G'_{\sigma}^{-1} - G_{\sigma}^{-1} = T(e^{V'_\sigma} - e^{V_\sigma}) + O(\Delta \tau^3/2)$ (note that $\alpha$ is of the order of $\Delta \tau^{1/2}$). On the other hand $T = (G_{\sigma}^{-1} - 1 - \Delta \tau^2 V^2 G_0) e^{-V_\sigma}$ which results

$$G'_{\sigma}^{-1} - G_{\sigma}^{-1} = (G_{\sigma}^{-1} - 1) e^{-V_\sigma} (e^{V'_\sigma} - e^{V_\sigma}) + O(\Delta \tau^{3/2}).$$

Multiplying from the left by $G$ and from the right by $G'$ and, ignoring terms $O(\Delta \tau^{3/2})$, we find

$$G'_\sigma = G_\sigma + (G_{\sigma} - 1)(e^{V'_\sigma} - e^{V_\sigma} - 1)G'_\sigma \text{ or } G_\sigma G'_\sigma^{-1} = 1 + (1 - G_\sigma)(e^{V'_\sigma} - e^{V_\sigma} - 1)$$

The QMC process proceeds by sequentially proposing changes in each Hubbard-Stratonovich (HS) field, accepting these changes with the transition probability $P_{s' \to s}$ of accepting a change from HS field configuration $\{s_l\}$ to $\{s'_l\}$. The probability of a configuration $\{s_l\}$ is $P_s \propto \det(G_{\{s_l\}}^{-1}) \det(G_{\{s_l\}}^{-1})$; on the other hand detailed balance requires $P_s P_{s' \to s} = P_{s'} P_{s' \to s}$ for all $s'$. We may satisfy this requirement either by defining the transition probability $P_{s' \to s} = R/(1 + R)$, where

$$R \equiv \frac{P_s}{P_{s'}} = \frac{\det(G'_{1}) \det(G'_{1})}{\det(G_{1}) \det(G_{1})}$$

is the relative weight of two configurations, or by letting $P_{s' \to s} = \text{minimum}(R, 1)$. The first choice defines the “heat bath” algorithm, and the second the Metropolis algorithm. In either case, if the change is accepted, then we must update the Green’s
function accordingly. If the difference between two configuration is due to a flip of a single Hubbard Stratonovich field at the $m$th imaginary time slice then\[28\]
\[
R = \prod_{\sigma} [1 + (1 - G_{\sigma,m})(e^{-\alpha \sigma(s_m - s'_m)} - 1)]^{-1}.
\]
\[
(43)
\]
Finally we can write down the evolution of the Green’s function in the QMC time as\[28\]
\[
G'_{\sigma,i,j} = G_{\sigma,i,j} + \frac{(G_{\sigma,i,m} - \delta_{i,m})(e^{-\alpha \sigma(s_m - s'_m)} - 1)}{1 + (1 - G_{\sigma,m,m})(e^{-\alpha \sigma(s_m - s'_m)} - 1)} G_{\sigma,m,j}.
\]
\[
(44)
\]
We now have all the equations necessary to construct an algorithm. We initiate this procedure by letting $G_{\sigma}(\tau, \tau') = \mathcal{G}(\tau - \tau')$ where $\mathcal{G}$ is defined in Sec. 2.1, and choosing the corresponding field configuration with all $s_l = 0$. We use Eq. 44 to create a Green’s function for a physically realistic field configuration (i.e., $s_l = 1$, for all $l$). We warm up the system by sequentially stepping through the time lattice, proposing changes at each site $s_l \rightarrow -s_l$. We accept the change if $P_{s_l -> -s_l}$ is greater than a random number between zero and one and update the Green’s function using Eq. 44 if the change is accepted. The warmup lasts for a few hundred lattice sweeps before measurements begin. Thereafter, we typically perform four complete lattice sweeps between measurements to produce more-or-less independent samples. We do not measure after each sweep since the measurement process is also cpu intensive. After several hundred or a thousand complete sweeps through the time lattice it is necessary to compensate for roundoff error accumulated in the the Green’s function through repeated use of Eq. 44. This is accomplished by setting $G(\tau, \tau') = \mathcal{G}(\tau - \tau')$ and using Eq. 44 repeatedly until the Green’s functions corresponds to the present HS field configuration. Since the bare Green’s function $\mathcal{G}$ is not \textit{a priori} known, the QMC algorithm must be iterated as shown in Fig. 3 to determine a self-consistent solution for the Green’s function of the infinite-dimensional lattice. This process is repeated until convergence is reached. If a reasonable approximate solution exists, then this may be used instead of the QMC for first few iterations to save cpu time. The values of $L$ used ranged from 8 to 160, with the largest values of $L$ reserved for the largest values of $\beta$ since the time required by the algorithm increases like $L^3$. Experience shows that no severe sign problem occurs in the QMC process for Hubbard-like models.

\subsection*{3.2 Making and Conditioning Measurements}

The natural byproduct of the QMC algorithm are the Green’s functions. These may be used to make measurements of most one and two-particle properties using standard diagrammatic techniques. In doing so, several points must be remembered:

- In the QMC algorithm, the Hubbard-Stratonovich transformation reduces the problem to one of free electrons moving in a time-dependent Hubbard-Stratonovich
field. Thus, for each field configuration, any diagram may be formed by sum-
ing all allowed Wick’s contractions. The full interacting quantity is recovered
by averaging this over all field configurations.

- It is important to use all allowed Wick’s contractions, both connected and
disconnected, in this series.

- In order to produce the lowest variance measurement, it is important to average
over all time differences.

- It is also important to average over all the symmetries of the Hamiltonian, which
may not be preserved by the action.

Thus, for example, for one HS field configuration the QMC local Green’s function has
the form

\[
G_\sigma = \left( \begin{array}{cccc}
G_\sigma(0+ , 0) & G_\sigma(0, \Delta \tau) & G_\sigma(0, 2\Delta \tau) & G_\sigma(0, 3\Delta \tau) \\
G_\sigma(\Delta \tau, 0) & G_\sigma(\Delta \tau+, \Delta \tau) & G_\sigma(\Delta \tau, 2\Delta \tau) & G_\sigma(\Delta \tau, 3\Delta \tau) \\
G_\sigma(2\Delta \tau, 0) & G_\sigma(2\Delta \tau, \Delta \tau) & G_\sigma(2\Delta \tau, 2\Delta \tau) & G_\sigma(2\Delta \tau, 3\Delta \tau) \\
G_\sigma(3\Delta \tau, 0) & G_\sigma(3\Delta \tau, \Delta \tau) & G_\sigma(3\Delta \tau, 2\Delta \tau) & G_\sigma(3\Delta \tau+, 3\Delta \tau) \\
\vdots & \vdots & \vdots & \vdots \\
\vdots & \vdots & \vdots & \vdots \\
\end{array} \right) \quad (45)
\]

Here, by convention, in the diagonal elements the first time index is taken to be later
than the second by an infinitesimal. When we average this over all HS field configura-
tions, the time-translational invariance is restored, so for example \( \langle G_\sigma(2\Delta \tau, \Delta \tau) \rangle \approx G_\sigma(\Delta \tau) \). So for each value of \( 0 \leq l\Delta \tau < \beta \) there are \( L \) estimates of \( G_\sigma(l\Delta \tau) \), and
if there is no external field and the simulation is in the paramagnetic state, then
\( G_\sigma(l\Delta \tau) = G_{-\sigma}(l\Delta \tau) \). Thus, the lowest variance estimator of the Green’s function
is obtained by averaging over all equivalent time differences and spin making sure
to account for the antiperiodicity of the Green’s function (i.e., \( \langle G_\sigma(2\Delta \tau, 3\Delta \tau) \rangle \approx
- G_\sigma((L - 1)\Delta \tau) \)).

Since the Hirsch-Fye algorithm requires an imaginary-time path integral technique
which only produces data for \( G(\tau) \) at a discrete set of points in Euclidean time \( 0 <
\tau < \beta \), estimation of the Matsubara frequency Green’s function requires a numerical
approximation of the integral

\[
G(i\omega_n) = \int_0^\beta d\tau e^{-i\omega_n \tau} G(\tau) . \quad (46)
\]

Fourier transforming discretely sampled data presents some well known difficulties[32].
The principle difficulty is formalized by Nyquist’s theorem which tells us that above
the frequency \( \omega_N = \frac{2\pi}{2\Delta \tau} \) unpredictable results are produced by conventional quadra-
ture techniques. For example, a rectangular approximation to the integral yields a
periodic $G(i\omega_n)$. This presents a difficulty since causality\cite{33} requires that

$$
\lim_{\omega_n \to \infty} G(i\omega_n) \sim \frac{1}{i\omega_n} .
$$

Typically this problem is overcome by fitting the discrete data $G(\tau)$ with a smooth knotted Akima spline\cite{34}, and then performing the integral on the splined data\cite{32}. Since the integral on the splined data may be sampled on a much finer grid than the original data, this process is referred to as oversampling.

However, a problem still remains at high frequencies, since the oversampled $G(i\omega_n)$ goes quickly to zero for frequencies above the Nyquist frequency. In order to maintain the proper high-frequency behavior of Matsubara frequency Green’s functions, we condition the Fourier transform with a perturbation theory result. That is, we write

$$
G(i\omega_n) = G_{pt}(i\omega_n) + \int_0^\beta d\tau e^{-i\omega_n \tau} (G(\tau) - G_{pt}(\tau)) .
$$

where $G_{pt}$ is a Green’s function obtained from perturbation theory, and the integral here is performed by the oversampling method described above.

There are two obvious advantages to this approach. First, the integral goes to zero for frequencies greater than the Nyquist frequency $\pi/\Delta \tau$, so that the resulting Green’s function has the same asymptotic behavior as the perturbation theory result, and is thus causal. Second, often, the perturbation theory result is asymptotically exact\cite{35} (i.e. results from a high temperature expansion etc.), and this then presents a way of appending exact QMC results at low frequency with asymptotically exact perturbation theory results at high frequency.

As another example, consider the local impurity magnetic susceptibility

$$
\chi(T) \approx \int_0^\beta d\tau \langle S^+(\tau)S^-(0) \rangle \\
\approx \int_0^\beta d\tau \langle C^\dagger_1(\tau)C_1(\tau)C^\dagger_1(0)C_1(0) \rangle \\
\approx \frac{T}{2} \sum_\sigma \int_0^\beta d\tau \int_0^\beta d\tau' \langle G_\sigma(\tau + \tau', \tau')G_{-\sigma}(\tau', \tau + \tau') \rangle_{\{s_l\}}
$$

where the $\{s_l\}$ subscript means that the Monte Carlo average over the Hubbard-Stratonovich fields is still to be performed, and in the last step in Eq. 49 we form all allowed Wick’s contractions and average over all equivalent time differences to reduce the variance of this estimator. This measurement is best accomplished by splitting it in two parts. First, we measure $\chi(\tau)$

$$
\chi(\tau) = \frac{T}{2} \sum_\sigma \int_0^\beta d\tau' \langle G_\sigma(\tau + \tau', \tau')G_{-\sigma}(\tau', \tau + \tau') \rangle_{\{s_l\}}
$$

by approximating the integral as a sum using a rectangular approximation. For $\tau > 0$

$$
\chi(\tau) \approx \frac{1}{2L} \sum_{\sigma,l'} \langle G_\sigma(ind(l + l'), l')G_{-\sigma}(l', ind(l + l')) \rangle_{\{s_l\}} ,
$$
where \( \text{ind}(l) \) is the smaller nonnegative value of either \( l \) or \( l - L \). For \( \tau = 0 \) the fact that we always store \( G_\sigma(l', l') = G_\sigma(\tau_l + 0^+, \tau_l') \) requires us to modify the measurement

\[
\chi(\tau = 0) \approx \frac{1}{2L} \sum_{\sigma, l'} \langle G_\sigma(l', l') (G_{-\sigma}(l', l') - 1) \rangle \{ s_i \} .
\]  

(52)

Finally, hitting the first step, the equation becomes

\[
\chi(\tau) = \int_0^\beta d\tau \chi(\tau) \approx \sum_l s f(l) \Delta \tau \chi(\tau_l),
\]  

(53)

where the Simpson factor \( s f(l) = 2\Delta \tau / 3 \) \((4\Delta \tau / 3)\) for odd (even) \( l \) is used to reduce the systematic error of the integral.

As a final example, consider the local magnetic susceptibility (two-particle particle-hole Green’s function) \( \chi(i\omega_n, i\omega_m) \) matrix shown on the bottom-left of Fig. 5 and used in Sec. 2.2 to calculate the lattice susceptibility. The two-particle Green’s functions are difficult to measure efficiently. To construct a Matsubara-frequency measurement of this quantity, we associate a factor of \( \exp(i\omega_1\tau) \) \((\exp(-i\omega_1\tau)\mathcal{C}_\tau(\tau)\) with the beginning (end) of each external leg and integrate over all \( \tau \), so that

\[
\chi(i\omega_n, i\omega_m) = \int_0^\beta d\tau_1 \cdots d\tau_4 \exp[i\omega_n(\tau_1 - \tau_2) - i\omega_m(\tau_3 - \tau_4)] \langle T_\tau C_\tau(\tau_1) C_\tau(\tau_2) C_\tau(\tau_3) C_\tau(\tau_4) \rangle .
\]  

(54)

For a particular configuration of the Hubbard-Stratonovich fields, the Fermions are noninteracting, thus the expectation value indicated by the angle brackets above may be evaluated in two steps. First, using Wick’s theorem, its value is tabulated for each field configuration \( \{ s_i \} \). Second we Monte Carlo average over these configurations. After the first step, the equation becomes

\[
\chi(i\omega_n, i\omega_m) = \left\langle \sum_{\tau_1} \cdots \sum_{\tau_4} \exp[i\omega_n(\tau_1 - \tau_2) - i\omega_m(\tau_3 - \tau_4)] G_1(\tau_1, \tau_1) G_1(\tau_3, \tau_2) \right\rangle \{ s_i \} .
\]  

(55)

To measure this on the computer, the integrals must be approximated by sums. Since the Green’s functions change discontinuously when the two time arguments intersect, the best applicable integral approximation is the trapezoidal approximation. Using this, we will run into Green’s functions with both time arguments the same \( G(j, j) \). This is stored as \( G(j^+, j) \) (i.e., it is assumed that the first time argument is slightly greater than the second); however, if we replaced the equal time Green’s function to be the average \( \{ G(j^+, j) + G(j, j^+) \} / 2 = G^+(j, j) - 1/2 \) then a trapezoidal approximation of the integrals results. If we call \( \mathcal{G} \), with 1/2 subtracted from its diagonal elements, \( \mathcal{G} \), then

\[
\chi(j, k) = \left\langle \left( \sum_{n, n'} \Delta \tau e^{i\pi n'(2j + 1)} \mathcal{G}_1(n, n) \Delta \tau e^{-i\pi n'(2k + 1)} \right) \left( \sum_{m, m'} \Delta \tau e^{-i\pi m'(2j + 1)} \mathcal{G}_1(m, m) \Delta \tau e^{i\pi m'(2k + 1)} \right) \right\rangle \{ s_i \} .
\]  

(56)
This measurement may be performed efficiently if the product of three matrices in
in each set of parenthesis is tabulated as two sequential matrix-matrix products and
stored before the direct product between the terms in parenthesis is calculated. When
done this way, the time required for this measurement scales like $\sim L^3$ rather than
$\sim L^4$ as would result from a straight-forward evaluation of the sums implicit in Eq. 57.

4 Application: the Hubbard Model

In this section we present results from the Hubbard model to illustrate the power
and versatility of the method. This section is not meant to be an exhaustive discussion
of the model, for this, we refer the reader to two reviews[15, 36]

4.1 Phase Diagram

Near half filling, the Hubbard charge fluctuations are suppressed by the strong
local correlation which may open a Mott gap for sufficiently large $U$, but the system
can still gain hybridization energy if spins on adjacent sites are antiferromagnetically
aligned. Thus, the Hubbard model is expected to demonstrate antiferromagnetism
near half filling and a Mott transition at half filling.
Magnetic Phase Transitions

At Half Filling the expected antiferromagnetism is seen through the divergence of the antiferromagnetic susceptibility, shown in Fig. 6 (throughout this section, we choose $t^* = \sqrt{4t^2\delta} = 1$ as our unit of energy). Furthermore, since each lattice site has an infinite number of near neighbors and the transition is driven by intersite correlations between weakly screened moments, we expect this transition to be mean-field-like, so that near the transition $\chi_{AF} \sim 1/|T - T_c|^1$. This behavior is illustrated in the inset. The antiferromagnetic transition temperature $T_N$ is plotted as a function of $U$ in Fig. 6(a). For small values of $U$, where the local spin moment is also small, we find that $T_N$ is exponentially small, consistent with perturbation theory [38]. For very large values of $U$, where the spin moment and antiferromagnetic exchange have saturated to their maximum values, one expects that the transition temperature will fall monotonically with increasing $U$, $T_N \sim 1/U [38]$. This is because the net antiferromagnetic exchange $dJ \sim t^2/U$ also decreases with increasing $U$. Thus, a peak in $T_N(U)$ for some intermediate value of $U$ is expected as seen in Fig. 6(a). For comparison we included in Fig. 6(a) $T_N(U)$ for the $d = 3$ Hubbard model as calculated by Scalettar et al.[37]. The shape and order of magnitude compare very well, although the $d = 3$ data always have slightly larger values. At least part of this discrepancy is a consequence of the different analytic structures of the free DOS in $d = 3$ and $d = \infty$.

In Fig. 6(b) the unscreened squared magnetic moment $\mu^2 = \langle (n_1 - n_1)^2 \rangle$, calculated at the transition $T = T_N$, is plotted versus $U$ when $\epsilon = 0$. For the half-filled model $\mu^2$ ranges from $\mu^2 = 0.5$ in the uncorrelated limit ($U = 0$), to $\mu^2 = 1$ in the strongly correlated limit ($U \rightarrow \infty$). Note that the peak in $T_N(U)$ occurs near the point where $\mu^2$ begins to saturate to one.

This algorithm[10] may be easily modified[39] to work below $T_N$ in the antiferromagnetic phase of the half-filled model. As shown in Fig. 7, when $T < T_N$ a gap develops in the density of states due to the doubling of the unit cell. This gap develops continuously, so that when $T \lesssim T_N$ thermally induced states make the DOS finite at the Fermi surface. The width of this gap, measured from $\omega = 0$ to the first peak, increases monotonically with the ordered moment $|n_1 - n_1|$ shown in the inset to Fig.7(a).

Away from half filling the transition temperature falls quickly with doping, $\delta = 1 - <n>$. Once the doping exceeds a certain value, the transition is to an incommensurate state, as indicated by the divergence of the susceptibility $\chi(x(q), T)$ at a value of $x > -1$. This behavior is illustrated in Fig. 8 when $U = 4$ and $\delta = 0.188$. The transition temperature may then be determined by extrapolating the inverse of the peak in the susceptibility, $1/\chi_{max}$, as shown in the inset. In Fig. 9, the corresponding transition temperatures are plotted as a function of doping for various values of $U$. The open symbols indicate that the first divergence of the susceptibility was antiferromagnetic ($x = -1$); whereas, the filled symbols indicate that the susceptibility diverges into an incommensurate state.
Mott Gap

For temperatures above $T_N$ at half filling when $U$ is greater than the bandwidth, the energy is minimized when each site is singly occupied. Here, every charge fluctuation requires an energy of roughly $U$ minus the bandwidth. As a result, one expects to see a correlation induced Mott-Hubbard gap in the center of the single-particle density of states defined by $N(\omega) = -1/2\pi \sum \text{Im} G(\omega + i0^+)$ for sufficiently large values of $U$. This is shown in Fig. 7(b), where $N(\omega)$ is plotted for several values of $U$ when $\beta = 7.2$, and $\delta = 0$.

As the Coulomb repulsion $U$ is increased from zero the broad central peak in the spectrum becomes narrower and is gradually suppressed while at the same time two side bands build up which are carrying the majority of the spectral weight. The central peak can be associated with a quasi-particle resonance, and the side peaks as usual with incoherent charge transfer on and off the site. As $U$ continues to rise, the spectrum begins to develop a pseudogap at zero frequency when $U > 3.4 \approx U_C$. The “critical” value $U_C$ increases with increasing temperature, and for $U > U_C$ the pseudogap grows linearly in $U$ and the DOS splits into upper and lower Hubbard bands; however, due to the Gaussian band tails, zero energy transitions between these bands are still possible (albeit extremely unlikely). For this reason, no Mott transition was observed at finite temperatures in the hypercubic model; although, as the temperature is lowered, $\mu^2(U)$ appears to develop a kink, indicating that a there is probably a zero-temperature Mott transition if the antiferromagnetism is suppressed by frustration. A finite-temperature transition is observed in Bethe lattice models with a finite-bandwidth[36].

We also searched for charge density wave and superconducting phases. As far as
we know, there is no mechanism to support a charge density wave in the positive-$U$ model, and the strong local correlation appears to suppress gapless superconductivity. Order parameters with a spatial gap must have a symmetry lower than the lattice and, as discussed in Sec. 2.2, have no vertex corrections which are needed to drive a finite-temperature transition. I.e. there are no dynamical intersite (spin) fluctuations which can mediate superconductivity in the infinite dimensional model. This leaves only superconductivity with a temporal gap, or odd-frequency superconductivity. However, as illustrated in Fig. 10, we also were unable to find an odd-frequency transition.

4.2 The Paramagnetic Phase Away from Half Filling

Away from half filling, as shown in Fig. 11(a), the paramagnetic system becomes a heavy metal characterized by a narrow peak of width $\approx T_0$ in the single-particle density of states near the Fermi surface [23]. The development of this peak is associated with screening of the local moments[23], as shown in the inset to Fig. 11(a). Hence, we associate the peak with the Kondo effect and its width $T_0$ with the Kondo scale[42]. $T_0$ may be defined by the local spin susceptibility $\chi(T = 0) = 1/T_0$[43], and $T_0 = 0.073$ for the results shown in Fig. 11.

The development of the Kondo peak is also associated with features in the self energy as shown in Figs. 11(b) and (c). For $T \ll T_0$, both the real and imaginary parts of the self energy acquire a Fermi liquid form

$$\text{Re}\Sigma(\omega + i0^+) = \text{Re}\Sigma(0) + \omega(1 - Z) + O(\omega^2),$$

$$\text{Im}\Sigma(\omega + i0^+) = -\Gamma + O(\omega^2),$$

(57)

Figure 8: The magnetic susceptibility for all $x(q)$ at various temperatures when $U = 4$ and $\delta = 0.188$. The susceptibility displays a peak at $x \approx -0.90$. As shown in the inset, the transition temperature ($T_c = 0.0148t^*$) was inferred from extrapolation of the peak inverse susceptibility. Figure from[41]
with $\Gamma \propto T^2$ for temperatures $T \ll T_0$ the characteristic low-temperature scale. [The effective Fermi temperature $T_0$ decreases to zero as half filling is approached whenever $U$ is larger than the critical value for the Mott gap \cite{43}, and the Fermi-liquid-theory form of Eq. 57 still holds for moderate temperatures, with the only change being $\Gamma \propto T$ for $T > T_0$.]. The quasi-particle renormalization factor is given by the slope of the low temperature self energy

$$ m^*/m = a^{-1} = 1 - \left. \frac{d \text{Re} \Sigma(\omega)}{d \omega} \right|_{\omega=0,T=0}. $$

(58)

Roughly $a^{-1} = 4$ for the results shown in Fig. 11(c). One may also calculate the Eliashberg quasi-particle renormalization factor as discussed by Serene and Hess\cite{45}, $Z_0(T) = 1 - \text{Im} \Sigma(i\omega_0)/\omega_0$. The two definitions are consistent at zero temperature so long as the self energy is analytic. As the temperature is reduced below $T_0$, $Z_0(T)$ saturates to a finite value, indicating the formation of a Fermi liquid. The zero temperature limit of $Z_0(T)$ may be estimated by extrapolation, and it also gives the effective mass for the quasi-particles of this Fermi liquid $m^*/m = a^{-1}(0) \approx 4$. For fixed $U > U_C$, the effective mass appears to diverge continuously as half filling is approached\cite{43}.

As the temperature increases $T \gtrsim T_0$ the Kondo peak begins to diminish, the slope of the real part of the self energy also is diminished, indicating a reduced mass, and the imaginary part of the self energy develops a distinct non-Fermi liquid character $\text{Im} \Sigma(\omega) \sim \omega$. Here, $Z_0(T)$ increases in a roughly log-linear fashion. This behavior $Z_0(T) \sim \ln(T)$ has been identified \cite{45} as a signal of marginal Fermi liquid behavior \cite{46}. Let us stress, though, that this special behavior appears only as a crossover
feature from a high- to a low-temperature regime and does not persist as an anomalous ground state! In the high temperature regime, \( T \gg T_0 \), the Kondo peak disappears and the physical properties no longer show scaling[23]. 

\[
1 - \left. \frac{d \text{Re} \Sigma(\omega)}{d\omega} \right|_{\omega=0} \approx Z_0(T) \to 1
\]

as in the free metal, whereas \( \text{Im} \Sigma(\omega) \) remains large at the Fermi surface, due to thermal fluctuations and significant scattering from unscreened spins.

4.3 Transport Anomalies

The strong temperature dependence of the self energy leads to very interesting anomalies in the resistivity and NMR shown in Fig. 12. Most prominent is the pronounced linear region in \( \rho(T) \) which increases with increased doping. The slope of this region is proportional to \( 1/\delta \) as shown in the inset to Fig. 12(a). At low temperatures, the resistivity becomes quadratic in temperature, indicative of a Fermi liquid. The thermal conductivity \( \kappa \) was also calculated; however it is not plotted, since to a very good approximation, it follows the Wiedemann-Franz law \( \kappa \propto T/\rho \). Figure 12(b) presents the results for the NMR relaxation rate \( (1/T_1) \). Here, too, a rather anomalous variation with both temperature and doping is found. A linear region in \( 1/T_1 \) develops as the doping increases, and the slope changes sign for \( \delta \approx 0.15 \). The doping dependence of \( 1/T_1 \) is reduced as the temperature increases, but does not disappear at the temperatures that can be reached by numerical analytic continuation.

Anomalies are also seen in the thermopower \( (S) \) and the Hall coefficient \( (R_H) \). Fig. 13 compiles the results for \( S \) (Fig. 13a) and \( R_H \) (Fig. 13b) for five different dopings as function of temperature. \( S \) becomes negative at low temperatures indicating
Figure 11: (a) The evolution of the density of states when $U = 4$ and $\delta = 0.188$. The development of a sharp peak at the Fermi surface is correlated with the reduction of the screened local moment $T\chi(T)$, as shown in the inset. Hence the development of the peak may be associated with a resonant Kondo screening of the spins.

The imaginary (b) and real (c) parts of the self energy for various temperatures when $U = 4$ and $\delta = 0.188$. Note that as the temperature is lowered, Im$\Sigma(\omega)$ becomes parabolic in $\omega$, indicating the formation of a Fermi liquid. However, for $T > T_0$ the self energy takes on the features of the non-Fermi liquid with Im$\Sigma(\omega) \approx \omega$. Figures from[44]

a crossover from electron-like to hole-like transport as the temperature is decreased. This sign change at intermediate temperatures is characteristic of correlated materials. The Hall coefficient, in Fig. 13b, is more interesting. It is positive for high temperatures, and displays a maximum at intermediate temperatures, followed by a strong decrease for lower $T$, eventually becoming negative (qualitatively similar features have been seen in simulations of the two-dimensional Hubbard model [47]). Interestingly, the position of the maximum is weakly sensitive to doping while, as shown in the inset, its height roughly decreases with increasing doping like $R_H \sim 1/\delta$.

The optical conductivity $\sigma(\omega)$ is another important probe of a strongly correlated system. It measures the rate at which electron-hole pairs are created by photons of frequency $\omega$. Figure 14 shows the results[44] for $\sigma(\omega)$ obtained from Eq. (6) when $\delta = 0.068$ for a variety of temperatures (a), and results for $\beta = 43.2$ and various dopings $\delta$ (b). The Drude peak at $\omega = 0$ develops with decreasing temperature. In addition there appears a small mid-infrared peak at $\omega \approx 1$. As shown in Fig. 14b,
Figure 12: (a) Resistivity versus temperature for several different dopings when $U = 4$. The slope in the linear regime, determined by a linear least squares fit, increases linearly with $1/\delta$ as shown in the inset. The units on the vertical axis are approximately $10^3 \Omega \cdot \text{cm}$.

(b) NMR relaxation rate $1/T_1$ vs. temperature for different dopings at $U = 4t^*$. The lines are linear fits in the anomalous region. Figure from[43]
	his peak is more pronounced for small $\delta$ but remains visible even at larger doping. In addition, it is strongly temperature dependent and clearly visible only for the lowest temperatures. We attribute it to excitations from the lower Hubbard band to the quasiparticle band at the chemical potential. The last feature in $\sigma(\omega)$ is a roughly temperature-independent peak at $\omega \approx U$ due to the charge excitations from the lower part of the spectrum, i.e., from the lower Hubbard band and the quasiparticle peak at $\mu$, to the upper Hubbard band (cf. Fig. 11).

The insets to Fig. 14 show the development of the Drude weight as obtained from Eq. (8) as a function of doping (Fig. 14b) and the width of the Drude peak as function of temperature (Fig. 14a). The latter was obtained by fitting the generic form

$$\sigma(\omega \to 0) = \frac{D \tau}{\pi \left(1 + \tau^2 \omega^2\right)}$$

(59)

to the low-frequency regions in Fig. 14a. The Drude weight initially increases linearly with $\delta$, then saturates to its maximal value at $\delta \approx 0.5$, before decreasing. This behavior can be understood in terms of a simple picture: The Drude weight is determined by the carrier density and effective mass via $D \propto n/m^*$. From the doping-dependence of the quasiparticle peak in the single-particle density of states[44] one may assume $m^{*-1} \propto \delta$. The carrier density, on the other hand, is given by $n \sim 1 - \delta$. 

Figure 13: Thermopower (a) and Hall coefficient (b) for five different dopings $\delta$ as function of temperature. In (a) the solid lines are from a fit to the QMC. In the inset to (a), the Hall coefficient at a fixed temperature $R_H(T = 0.19)$ is plotted versus $1/\delta$, indicating that $R_H$ near the peak increases roughly in proportion to $1/\delta$. The units on the vertical axis are approximately $86\mu V/K$ for the thermopower (a) and $10^{-9} m^3/C$ for $R_H$ (b). Figure from [15].

i.e. $D \propto \delta(1 - \delta)$. This expression explains the behavior for small doping as well as the maximum, which should lie at $\delta_{\text{max}} \approx 0.5$, and explains how the character of the carriers changes from being holelike near half filling to being electronlike at low density.

The width of the Drude peak, $1/\tau$, displays a linear behavior $1/\tau \sim T$ for $T \lesssim 0.1$. This dependence may be traced back to the development of the Kondo peak below $T_0$. Note that the intercept of the linear region does not lead to $1/\tau \to 0$ as $T \to 0$ as required, implying that for very low temperatures the Drude width decreases more rapidly ($1/\tau \sim T^2$), as expected for a Fermi liquid.

Perhaps these anomalies in the transport should not seem surprising, since they are connected to the small energy scale $T_0$, which does not exist in normal Fermi-liquid metals. Furthermore, the Hubbard Hamiltonian [1] is usually considered the simplest model that contains at least some of the anomalous features of the high-$T_c$ superconductors [2]. These anomalies include a resistivity and NMR rate $1/T_1$ which increase linearly with temperature, the slope of the NMR rate changes sign with doping whereas that of the resistivity increase like the inverse of the doping and the Hall coefficient changes sign with doping and the value at the maximum increases like $1/\delta$. The optical conductivity shows a doping and temperature-dependent mid-IR peak and a Drude width that increases linearly with temperature. We find that the
Figure 14: (a) Optical conductivity vs. $\omega$ for various temperatures when $\delta = 0.068$. Note that at low temperatures, when the Kondo peak becomes pronounced in the DOS, a mid-IR feature begins to appear in $\sigma(\omega)$. As shown in the inset, if we fit this data to a Drude form, then the width of the Drude peak is found to increase roughly linearly with $T$.

(b) Filling dependence of the optical conductivity when $U = 4$ and $\bar{\gamma} = 43.2$. Note that for larger $\delta$ the mid-IR and Drude peaks begin to merge, so that the latter is less distinct. The inset shows the evolution of the Drude weight $D$ as a function of doping. $D$ is determined by the extrapolation method of Ref. [19]. Figure taken from[44].

infinite-dimensional Hubbard model for $T \gtrsim T_0$ exhibits strikingly similar anomalies. Furthermore is not surprising that at temperatures $T > T_0$, far from any transition, our dynamical mean-field result reproduces results expected of the two-dimensional model. However, at lower temperatures, dimensionality, which influences the nature of any phase transition present, becomes crucial. As mentioned in Sec. 2.2 superconductivity of lower symmetry than s-wave is not possible in the infinite-dimensional limit, and the effect of localization also cannot be captured, since $d = 2$ is the lower and $d = 4$ is the upper critical dimension for localization. Thus, we would not expect the infinite-dimensional Hubbard model to be able to capture the low-temperature physics of the two-dimensional material.

It is interesting to speculate about the excitations responsible for these anomalies. Given that non-local dynamical correlations are suppressed in the infinite-dimensional limit, one may eliminate all excitations except local spin and charge excitations as candidates. Since the latter occur at relatively large energy scales ($\sim U$), charge fluctuations may also be eliminated, leaving only the local spin fluctuations, i.e. Kondo screening, as the scattering mechanism responsible for the transport anomalies. Transport anomalies due to Kondo screening are not unusual. They are respon-
sible for the anomalous transport seen in dilute magnetic alloys, and heavy Fermion
metals. However, since in the Hubbard model each lattice site is embedded in a band
consisting only of similar correlated sites, the self consistency causes a strong normal-
ization of the site’s environment. This strong renormalization causes the transport
in the Hubbard model to be quite different than that seen in the Periodic Anderson
model.

5 Conclusion

Conventional methods of computational physics, such as QMC and exact diagonal-
ization, are often restricted to relatively small systems, and display technical problems
like the sign-problem. These difficulties make calculations and interpretations diffi-
cult, especially in the interesting parameter regimes of low temperatures and strong
electronic correlations. Our method of combining the simplifications arising in the
limit of \(d \to \infty\) with standard QMC techniques overcomes most of these difficulties
at the expense of moving the calculation into infinite dimensions. Thus for properties
where dimensionality is crucial, i.e. to study the detailed nature of the phase transi-
tion, or transitions driven by dynamical intersite correlations, conventional finite-sized
techniques should be applied. Where dimensionality is less important, i.e. to obtain
the rough outline of the phase diagram or to study the dynamics and thermodyna-
mics of the system in a regime far from any phase transition, then we believe that our
technique provides an attractive alternative.

As an example, we applied this method to the single-band Hubbard model, Eq.
1. In contrast to various approximate methods, our solution shows all the expected
features – an antiferromagnetically ordered ground-state close to half filling, and a
metal-insulator crossover at half filling – while retaining the essential dynamics in-
duced by the local correlations. Especially this last feature led to new and unexpected
results away from half filling, namely some sort of self-consistent “Kondo-effect” that
yields quite anomalous transport properties[15]

We have also applied this method to the periodic Anderson[48] and Holstein[49]
modes, and demonstrated that they also retain the properties expected of their three-
dimensional counterparts. In more recent simulations of the two-channel Kondo
lattice[50], we find a rich variety of behaviours, including non-Fermi liquid low-
temperature metallic state with a large residual resistivity, a first-order transition to
an odd-frequency superconducting state, as well as antiferromagnetism[50]. We be-
lieve that this new approach represents a powerful method to solve strongly correlated
lattice models and that most of our results will persist even for finite dimensionality.

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References


33. Causality is crucial when Bayesian methods are used to analytically continue QMC data, since the form of the Bayesian prior is dictated by causality.


42. The width of the peak is actually several times $T_0$, consistent with width of the Kondo resonance in the single-impurity Anderson model. See for example, H.O. Frota and L.N. Oliveira, Phys. Rev. B 33, 7871 (1986).


