A NEW APPROACH TO DOPED MOTT INSULATORS

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Abstract

We describe a new microscopic approach for analyzing interacting electron systems with local moments or, in principle, any local order parameter. We specialize attention to the doped Mott insulator phase of the Hubbard model, where standard weak–coupling perturbation methods fail. A rotationally invariant Stratonovich–Hubbard field is introduced to decouple the static spin components of the interaction at each site. Charge degrees of freedom are then treated by “slave” Hartree–Fock in the presence of a spatially varying random spin field. The effective action reduces to a classical Heisenberg model at half filling, insuring that the system has (i) finite–range order at \( T > 0 \) with an exponentially diverging correlation length and (ii) a one–electron Mott–Hubbard gap in the presence of disorder. Away from half–filling properties are determined by strongly non–Gaussian fluctuations in the amplitude and orientation of the local spin fields. The saddle point equations of the theory at zero temperature reduce to inhomogeneous Hartree–Fock, so that disordering of domain walls at finite temperature is in principle included. We present preliminary small system results for the intermediate and large interaction regimes obtained by Monte Carlo simulation of random spin field configurations.
1 Introduction

In this paper we describe a new approach to perturbation theory for systems with local moments or, in principle, any local order parameter. We begin by summarizing the present status of weak–coupling perturbation theories for such systems, with the Hubbard model as a primary example.

Over the course of the last decade weak–coupling perturbation theories have been used extensively to investigate the physics of the Hubbard model and its extensions. The simplest perturbative approach to the Hubbard model is just Hartree–Fock theory for one–body correlation functions. The conserving approximation implied for two–body correlations is then the random phase approximation, or RPA. In the large–$U$ limit at half–filling the static spin response is unstable within Hartree–Fock, and the system exhibits a broken–symmetry ground state with infinite–range antiferromagnetic order [1]. Furthermore a gap of order $U$ appears in the one–body density of states for the ordered phase. If the Hartree–Fock equations are extended to finite temperature, long–range antiferromagnetic order onsets at a temperature of order $U$ in the large–$U$ limit. The zero–temperature behavior of the Hartree–Fock approximation away from half–filling has also been investigated, and incommensurate states, as well as vertical and diagonal domain walls, have been studied [2]. However, the appropriate treatment for finite temperatures has remained unclear, because the energetic competition of the various states is delicate.

In fact the Hartree–Fock approximation at finite temperatures provides only a crude description of the physics in a two– (or one–) dimensional system. In accordance with the Mermin–Wagner Theorem [3], infinite–range magnetic order is forbidden for $T > 0$ in two dimensions. The magnetic correlation length $\xi(T)$ instead diverges exponentially in $1/T$ for $T \to 0$ at half–filling, and the quantitative behavior of $\xi$, as well as the zero–temperature ordered moment, is renormalized by quantum fluctuations. Nevertheless the half–filled model exhibits a gap (or pseudogap, since we do not mean to imply a rigorously zero density of states) at finite temperature in the spin–disordered phase.

With the intention of modeling strong spin fluctuations in a disordered system, the present authors proposed the fluctuation exchange, or FLEX, approximation [4, 5, 6] as a plausible starting point. The self–consistent treatment of spin fluctuations in the one–body self–energy suppresses the magnetic ordering transition to zero temperature. Nevertheless the new approximation is itself flawed: It does not produce a sharp gap at half–filling and instead smears out the density of states, leaving a finite weight at zero energy for all temperatures [3, 4, 7]. Furthermore the spin response function diverges with decreasing temperature in a way which only roughly mirrors the exact behavior of the model. The failure at half–filling calls into question results obtained for large $U$ at small doping, and in the end the FLEX approximation fails to describe the pseudogap regime.

The inadequacy of the FLEX approximation has motivated various attempts to improve the theory. Kampf and Schrieffer have calculated the electron spectral density
near an antiferromagnetic transition to lowest order in an effective spin–fluctuation interaction, and their results exhibit a pseudogap when the spin correlation length is large [8]. Vilk and Tremblay [9] have introduced a factorization approximation for the electron four–point function which is constrained to be exact when all space–time coordinates coincide. Others [10] have argued that perturbative calculations based on an unrenormalized electron propagator are justified by a cancellation between vertex corrections and self–energies, leading to the appearance of a pseudogap in some parameter regimes.

In addition efforts have been made to extend the FLEX approximation within a scheme based on infinite–order (or “parquet”) vertex renormalization [11, 12, 13]. Quantitative studies of parquet renormalization have had the goal of establishing the validity or inadequacy of perturbation theory resummations for systems with a gap, but without infinite–range order. Why would one assume that such resummations have any chance of succeeding? For at least one nontrivial model, the Anderson impurity in a metallic host, it has been known since the mid–1980’s that zero–temperature perturbation theory for thermodynamic properties has an infinite radius of convergence in \( U \) [14]. This fact, as well as some suggestive results in the low–density limit, initially encouraged hope that an infinite–order parquet summation for the doped Mott insulator might succeed if the technical difficulties impeding its implementation could be overcome.

In fact this hope is not justified. Full numerical solutions of the minimal parquet equations for the two–dimensional Hubbard model in the large–\( U \) limit [15] yield the following results: (i) No gap appears in the converged solution at half filling. (ii) The spectral density at low energies is actually larger than that in a FLEX calculation. We interpret these results to mean that conventional perturbation theory [16] fails to describe the physics of a Mott–Hubbard gap or pseudogap in a spin–disordered system. Furthermore the parquet results, which consistently incorporate vertex renormalization to infinite order, bring into question whether the basic problem can be circumvented by the constrained factorization approximation or a cancellation between parts of perturbative diagrams.

Rather we believe the failure of perturbation theory around a uniform (i.e., Fermi liquid) starting point is due to a qualitative change in the saddle–point structure of the action for the Hubbard model at temperatures of order \( U \) in the large–\( U \) limit. This change is induced by the appearance of local moments (or, more generally speaking, a local order parameter field) in the theory. Conventional perturbation theory becomes unreliable below a temperature scale which depends on both the interaction \( U \) and the chemical potential \( \mu \). Below this scale one needs a revised perturbation theory which incorporates “anomalous” Feynman graphs, but does so without inducing infinite–range order. These seemingly contradictory objectives may be accomplished by introducing a spatially varying static field with the full symmetry of the associated classical order parameter. One way to introduce such a field is via a Stratonovich-Hubbard (S–H) transformation [17, 18] of the interaction. In particular we employ below a spin–rotation–invariant S–H field to decouple the static (\( m = 0 \))
component of the Hubbard interaction. About thirty years ago Wang et al. showed for the magnetic alloy problem that the effective static free energy induced by a time–varying S–H field provides a physical picture of the crossover from band–like to local–moment behavior. Evenson et al. analyzed the coupling between isolated moments which arises within this approach and noted that the simplest scheme generates an Ising, rather than Heisenberg, interaction. Below we show that when a vector S–H field is introduced, the effective action reduces to a classical Heisenberg form at half–filling. This means no infinite–range order at \( T > 0 \), an exponentially diverging correlation length \( \xi(T) \), and a Mott–Hubbard gap in the spin–disordered phase. Furthermore the approximation scheme should provide a systematic way to study doping of the Mott insulator. In the doped case both orientation and amplitude fluctuations of the field become important. In particular the effective action for the static field is strongly non–Gaussian. Since the action arises directly from integrating out the fermion degrees of freedom, its form reflects both the underlying spin and charge structure of the system. In this way domain wall stripe fluctuations can occur naturally if they are present in the model.

We describe this new approximation scheme for the Hubbard model in Section 2, then derive expressions for specific electron correlation functions in Section 3. In Section 4 we provide a brief description of our Monte Carlo sampling scheme for integration over the fluctuating local fields. In Section 5 we present some illustrative results obtained on a work station for a 4 \( \times \) 4 system. We outline in Section 6 the form of generalized approximations which extend the present approach in the same sense that FLEX extends Hartree–Fock. Finally we close in Section 7 with some speculations on possible implications for high–temperature superconductivity and with an outline of the next steps in this work.

2 Approximation scheme

In this section we show how to decouple the static spin interaction in the repulsive Hubbard model by introducing a spin–rotation–invariant S–H field. This field may be interpreted as a classical Heisenberg order parameter which generalizes the saddle–point in conventional temperature–dependent Hartree–Fock calculations.

It is conventional to decouple the interaction term by introducing independent fields at each point in imaginary time. When this is done, some freedom remains in choosing the form of the interaction, due to the equal–time fermion anticommutation relations. One may write equivalently

\[
U \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} = \frac{1}{4} U (\hat{n}_i^2 - \hat{m}_{iz}^2) \tag{1}
\]

\[
= \frac{1}{2} U (\hat{n}_i - \hat{m}_{iz}^2) \tag{2}
\]

\[
= \frac{1}{2} U \hat{n}_i - \frac{1}{4} U (\hat{m}_{iz}^2 + \hat{m}_{iy}^2) \tag{3}
\]

where

\[
\hat{n}_i = \hat{n}_{i\uparrow} + \hat{n}_{i\downarrow}
\]
The z-component of the moment operator in Eqns. 1 and 2 may be replaced by the x- or y-component, and likewise different pairwise combinations of moment operators may be substituted in Eqn. 3. One is free to consider in addition arbitrary linear combinations of these expressions, weighted properly to reproduce the original interaction.

This was realized by several authors around 1970 during early studies of the single-impurity Anderson model and the Hubbard model. In particular Wang et al. employed Eqn. 2 \[19\] and Hamann employed Eqn. 1 \[22\] as the starting points for equal-time Stratonovich-Hubbard decoupling schemes. Note that both these expressions imply an Ising-like S–H field governing the spin degrees of freedom, while the third expression implies an xy-like field. All three expressions result in actions which break the spin–rotational symmetry of the theory, and the symmetry is only restored by the integration over field configurations. As long as all configurations are included there is no difficulty, but problems arise if approximations are introduced for any system beyond a single impurity. This was realized by Evenson et al. \[20\] in large-U studies of the two-site Hubbard model within a static approximation: The effective spin–spin coupling assumes an Ising, rather than Heisenberg, form when Eqn. 2 is used as a starting point. It would clearly be desirable to introduce a symmetrical Heisenberg decoupling, but this is difficult for the following reason: No matter how the spin quantization axis is chosen, the three equivalent components of the spin–spin interaction are divided up between the two particle-hole channels (longitudinal and transverse) of the electron vertex, which “overlap” completely at equal time. A Heisenberg decoupling can be introduced artificially if, for example, the interaction is written as an equal-weight linear combination of Eqn. 1 for the three choices of moment operator, i.e.,

\[
U \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} = \frac{1}{4} U \hat{n}_i^2 - \frac{1}{12} U \hat{m}_i \cdot \hat{m}_i .
\]  

(5)
independent of the expression employed for the interaction in Eqs. (6). The same
procedure can be applied in more general situations when it is necessary to decouple
multiple interactions in crossed channels.

It is possible to carry out this transformation directly within an operator–based ap-
proach, but the manipulations are more transparent with anticommuting c–numbers,
and we follow the latter approach. We consider a discretized representa-
tion of the partition function
\[ Z = \text{Tr} e^{-\beta \hat{H}}, \]  
where
\[ \hat{H} = -t \sum_{\bar{i}d\sigma} c_{\bar{i}+\delta,\sigma}^\dagger c_{i\sigma} + U \sum_i c_{i\uparrow}^\dagger c_{i\downarrow} c_{i\uparrow} c_{i\downarrow} - \mu \sum_{i\sigma} c_{i\uparrow} c_{i\sigma}. \]  
Let
\[ \tau_{\ell} = \ell \Delta \tau \]
\[ \Delta \tau = \beta / L, \]  
with \( L \) the number of time slices. We write the anticommuting c–numbers for time
\( \tau_{\ell} \), site \( i \), and spin \( \sigma \) as \( c_{\ell i\sigma}^\dagger, c_{\ell i\sigma} \). It is convenient to use the frequency–transformed
variables \( \tilde{c}_{n\sigma}^\dagger, \tilde{c}_{n\sigma} \), where
\[ \tilde{c}_{n\sigma}^\dagger = \sum_{n=-L/2}^{L/2-1} e^{i\omega_n \tau_{\ell}} c_{\ell i\sigma}^\dagger \]
\[ \tilde{c}_{n\sigma} = \sum_{n=-L/2}^{L/2-1} e^{-i\omega_n \tau_{\ell}} c_{n\sigma} \]  
with
\[ \omega_n = (2n + 1)\pi T \]  
for integer \( n \). In order to keep track of discretization effects, we define
\[ i\omega_n^\Delta \equiv \frac{1 - e^{-i\omega_n \Delta \tau}}{\Delta \tau}, \]  
which approaches \( i\omega_n \) for \( \Delta \tau \to 0 \).

The discretized fermion action is
\[ S = -\beta \sum_{in\sigma} (i\omega_n^\Delta + \mu) \tilde{c}_{n\sigma}^\dagger \tilde{c}_{n\sigma} + \beta \sum_{ibn\sigma} (-t) \tilde{c}_{b+\delta,\sigma}^\dagger \tilde{c}_{i\sigma} + \beta U \sum_{imn+m'} \tilde{c}_{n+m\uparrow}^\dagger \tilde{c}_{n-1\uparrow} \tilde{c}_{n'\downarrow} \tilde{c}_{n'+m\downarrow}. \]  
The interaction term is represented in Figure 1. (Note that the integer label \( -n - 1 \)
corresponds to frequency \( \omega_{-n-1} = -\omega_n \).) Equivalently one may write
\[ S = S_0 + S_{\text{int}}, \]
with

\[ S_0 = \beta \sum_{ijns} \epsilon_i^\sigma n \left[ -i \omega_n^s A + (H_0 - \mu \bf{1}) \right] \epsilon_j^\sigma, \]

where the matrix in brackets has spatial indices, and

\[ 1_{ij} = \delta_{ij}, \quad (H_0)_{ij} = \begin{cases} -t, & i \text{ and } j \text{ near-neighbors} \\ 0, & \text{else.} \end{cases} \]

Now note that the interaction can be rewritten in two equivalent ways to emphasize the particle–hole channels (see Figures 2a–b):

\[ S_{\text{int}} = -\beta U \sum_{mnn'} c_{i+m} n \epsilon_{i} c_{i} n \epsilon_{i} + \beta U \sum_{mnn'} c_{i+m} n \epsilon_{i} c_{i} n \epsilon_{i}. \]

At this stage we restrict attention to terms with \( m = 0 \), i.e., the static component of the particle–hole interactions. For \( m = 0 \) the two sums in Eqn. (16) are essentially independent: The only terms which appear in both sums are restricted to \( n' = n \). Therefore the static particle–hole interaction may be written

\[ S_{\text{int}}^{m=0} = -\beta U \sum_{i} \left[ \sum_{n} \epsilon_{i} c_{i} n \epsilon_{i} \right] \left[ \sum_{n'} \epsilon_{i} c_{i} n \epsilon_{i} \right] + \beta U \sum_{i} \left[ \sum_{n} \epsilon_{i} c_{i} n \epsilon_{i} \right] \left[ \sum_{n'} \epsilon_{i} c_{i} n \epsilon_{i} \right]. \]

where we have dropped from the double sums an \( n' = n \) correction term, which becomes negligible at low temperatures \[23\].

Now all terms in Eqn. (17) may be reduced to sums of perfect squares in preparation for the introduction of S–H fields. First note that

\[ \sum_{n} \epsilon_{i} c_{i} n \epsilon_{i} = \frac{1}{2} \sum_{n} \epsilon_{i} \left( \sigma_x + i \sigma_y \right)_{\alpha \alpha'} c_{i} n \epsilon_{i} \]

\[ \sum_{n} \epsilon_{i} c_{i} n \epsilon_{i} = \frac{1}{2} \sum_{n} \epsilon_{i} \left( \sigma_x - i \sigma_y \right)_{\alpha \alpha'} c_{i} n \epsilon_{i}. \]

Using these identifications one has

\[ \left[ \sum_{n} \epsilon_{i} c_{i} n \epsilon_{i} \right] \left[ \sum_{n'} \epsilon_{i} c_{i} n \epsilon_{i} \right] = \frac{1}{4} \left[ (m_{\alpha 0}^i)^2 + (m_{y 0}^i)^2 \right]. \]

where

\[ m_{\alpha 0}^i = \sum_{n} \epsilon_{i} \left( \sigma_x \right)_{\alpha \alpha'} c_{i} n \epsilon_{i}, \]

\[ m_{y 0}^i = \sum_{n} \epsilon_{i} \left( \sigma_y \right)_{\alpha \alpha'} c_{i} n \epsilon_{i}. \]
Likewise,
\[
\sum_n \sigma_n^\uparrow \sigma_n^\downarrow = \frac{1}{2} (n_0^\uparrow + m_{z_0}^\uparrow)
\]
\[
\sum_n \sigma_n^\downarrow \sigma_n^\uparrow = \frac{1}{2} (n_0^\downarrow - m_{z_0}^\downarrow),
\]
where
\[
n_0^i = \sum_n (\sigma_n^\uparrow \sigma_n^\downarrow + \sigma_n^\downarrow \sigma_n^\uparrow)
\]
\[
m_{z_0}^i = \sum_{n\alpha\alpha'} \sigma_n^{\alpha\alpha'} (\sigma_\alpha^z)_{\alpha\alpha'} c_n^{i\alpha'}.
\]

In this case one identifies
\[
\left[ \sum_n \sigma_n^\uparrow \sigma_n^\downarrow \right] \left[ \sum_n \sigma_n^{\downarrow} \sigma_n^{\uparrow} \right] = \frac{1}{4} \left[ (n_0^\uparrow)^2 - (m_{z_0}^\uparrow)^2 \right].
\]
Thus
\[
S_{m=0}^{\text{int}} = \frac{1}{4} \beta U \sum_i (n_0^i)^2 - \frac{1}{4} \beta U \sum_i (\vec{m}_0^i \cdot \vec{m}_0^i)^2.
\]

The repulsive charge interaction is retained for treatment by perturbation theory (i.e., saddle–point plus fluctuations). The attractive spin interaction in Eqn. (24) may be decoupled using an independent static S–H field at each site \(i\):
\[
\text{exp} \left[ -S_{\text{spin}}^{m=0} \right] = \text{exp} \left[ \frac{1}{4} \beta U \sum_i (n_0^i)^2 - \frac{1}{4} \beta U \sum_i (\vec{m}_0^i \cdot \vec{m}_0^i) \right]
\]
\[
= \int \prod \left( \frac{\beta}{\pi} \right)^{3/2} d\xi_x^i d\xi_y^i d\xi_z^i \exp \left[ -\beta \sum_i \vec{\xi}_i^i \cdot \vec{\xi}_i^i + \beta \sqrt{U} \sum_i \vec{\xi}_i^i \cdot \vec{m}_0^i \right].
\]

The S–H fields \(\vec{\xi}_i^i\) may be interpreted as classical magnetic fields which couple to the local electron spin polarization. The Hubbard action may be rewritten as
\[
S = \beta \sum_i |\xi_i^i|^2 + \tilde{S}_0 + S_{\text{charge}}^{m=0} + S_{\text{int}}^{m=0},
\]
where
\[
\tilde{S}_0 = \beta \sum_{ij\alpha\alpha'} \sigma_n^{\alpha\alpha'} \left\{ -i\omega_n^\Delta \delta_{\alpha\alpha'} \delta_{ij} + \left[ (H_0)_{ij} \delta_{\alpha\alpha'} - \sqrt{U} \vec{\xi}_i^i \cdot \vec{\sigma}_{\alpha\alpha'} \delta_{ij} - \mu \delta_{ij} \delta_{\alpha\alpha'} \right] \right\} c_n^{i\alpha'}
\]
and
\[
S_{\text{charge}}^{m=0} = \frac{1}{4} \beta U \sum_i (n_0^i)^2.
\]

The interaction contributions to the action for \(m \neq 0\) take precisely the form they would in a conventional perturbative treatment, except that all vertices related to
the zero–frequency spin vertex by crossing are absent. Note that because we have decoupled only the \( m = 0 \) spin components, we have left open the possibility of higher order perturbative expansions about a static approximation.

We consider now the static charge interaction \( S_{\text{charge}}^{m=0} \) in Eqn. \( \text{[23]} \). This term could be decoupled in parallel with \( S_{\text{spin}}^{m=0} \) by introducing a real–valued S–H field \( \rho^i \). Since the charge interaction is repulsive, however, the fermion bilinear coupling to \( \rho^i \) would be pure imaginary and unsuitable for Monte Carlo simulation. It is straightforward to show that a saddle–point approximation for the \( \rho^i \) fields in the presence of a fixed \( \vec{\xi}^i \) configuration yields the same result as a spatially non–uniform Hartree–Fock. For this reason we do not introduce \( \rho^i \) fields, but reserve \( S_{\text{charge}}^{m=0} \) for treatment by perturbation theory (i.e., Hartree–Fock at lowest order).

Within such a Hartree–Fock approximation for fixed \( \vec{\xi}^i \),

\[
S_{\text{charge}}^{m=0} \to \frac{1}{2} \beta U \sum_{i\alpha} \langle n^i \rangle_\xi \tilde{\tau}^\alpha_n c^\dagger_n - \frac{1}{4} \beta U \sum_i \langle n^i \rangle_\xi^2 ,
\]

where \( \langle n^i \rangle_\xi \) is the mean occupancy at site \( i \). It is essential to retain the “constant” term, since it depends on the local field configuration \( \{ \vec{\xi}^i \} \). From this point we use the notation \( \langle A \rangle_\xi \) to denote the expectation value of the fermion observable \( A \) in the presence of a fixed field configuration.

The static \( \vec{\xi} \)-dependent action assumes the form

\[
\bar{S}(\xi) = \bar{S}_0(\xi) + \bar{S}_f(\xi, \tau, c) ,
\]

where

\[
\bar{S}_0(\xi) = \beta \sum_i |\xi^i|^2 - \frac{1}{4} \beta U \sum_i \langle n^i \rangle_\xi^2 \\
\bar{S}_f(\xi, \tau, c) = \beta \sum_{ij\alpha\alpha'} \tau^\alpha_n \left\{ -i\omega_n \delta_{ij} \delta_{\alpha\alpha'} + \left[ (H_0)_{ij} \delta_{\alpha\alpha'} - \sqrt{U} \vec{\xi}^i \cdot \vec{\sigma}_{\alpha\alpha'} \delta_{ij} \\
+ \left( \frac{1}{2} U \langle n^i \rangle_\xi - \mu \right) \delta_{ij} \delta_{\alpha\alpha'} \right\} c^\dagger_{n}^\alpha \).
\]

The fermion contribution to the action may now be integrated out exactly, since it takes a one–body form (albeit a form non–diagonal in spin):

\[
\int D\tau \, Dc \, \exp[-\bar{S}_f] = \prod_r \left[ 1 + e^{-\beta \varepsilon_r(\xi)} \right] ,
\]

where the \( \varepsilon_r \) are eigenvalues of the one–body Hamiltonian

\[
H(\xi) = -t \sum_{\delta\alpha} \sum_{\alpha\alpha'} c^\dagger_{\delta\alpha} c_{\alpha\alpha'} - \sqrt{U} \sum_{i\alpha\alpha'} \vec{\xi}^i \cdot \vec{\sigma}_{\alpha\alpha'} c_{i\alpha}^\dagger \vec{\sigma}_{\alpha\alpha'} c_{i\alpha} + \sum_i \left[ \frac{1}{2} U \langle n^i \rangle_\xi - \mu \right] c^\dagger_{i\alpha} c_{i\alpha} .
\]

Thus the final expression for the effective action after the fermion integration is

\[
S_{\text{eff}}(\xi) = \bar{S}_0(\xi) - \sum_r \log \left[ 1 + e^{-\beta \varepsilon_r(\xi)} \right] .
\]
Note that for fixed $\mu$ and $\vec{\xi}_i$ a Hartree–Fock iteration is required to adjust the non–uniform charge field $\langle n^i \rangle$ to satisfy the condition

$$\langle n^i \rangle = \sum_r f(\varepsilon_r) \sum_{\sigma} |\langle r|i\sigma \rangle|^2$$

$$f(\varepsilon_r) = \frac{1}{1 + e^{\beta\varepsilon_r}}.$$  \hspace{1cm} (35)

In this equation $|r\rangle$ is the one–body eigenvector corresponding to eigenvalue $\varepsilon_r(\xi)$; and the $|i\sigma\rangle$ constitute a complete set of basis vectors corresponding to spin $S_z = \sigma$ on site $i$. Note that for an $N_{\text{sites}} \times N_{\text{sites}}$ real–space lattice, the size of the eigenvector space is $2^{N_{\text{sites}}}$. 

The form of the charge–interaction Hartree–Fock employed here provides a template for the family of Baym–Kadanoff \cite{24} (or FLEX \cite{2}) generalizations of the present approach discussed in Section 6. The charge field is here viewed as a nonsingular “slave” to the spin field: It is fixed to its saddle–point, which changes when the $\xi$ configuration changes.

No further approximation to the action $S_{\text{eff}}(\xi)$ is now possible without explicitly breaking spin rotational and translational invariance. In conventional Hartree–Fock treatments it is assumed that the static field $\vec{\xi}_i$ assumes a rigid configuration. At half–filling the mean–field ansatz is just

$$\langle n^i \rangle = \mid \vec{\xi} \rangle = \vec{\xi} e^{iQ \cdot R_i}, \hspace{1cm} Q = (\pi, \pi)$$

A saddle–point evaluation of $S_{\text{eff}}$ within this restricted field space reproduces the conventional Hartree–Fock equations for a commensurate antiferromagnet. Furthermore inhomogeneous Hartree–Fock solutions \cite{2} for $\langle n \rangle \neq 1$ follow by assuming a spin–space form (collinear, spiral, etc.) for the order parameter and solving the resulting saddle–point equations.

We propose instead to evaluate electron correlation functions using $S_{\text{eff}}$ as the action in a classical field Monte Carlo. The Monte Carlo is classical since all finite–frequency contributions to the action have been set aside for treatment by perturbation theory: Such contributions, when included, alter the form of the static field action, but are not themselves statistically sampled. By this means it is possible to insure that higher–order approximations have a positive–definite weighting factor $\exp(-S_{\text{eff}})$, avoiding the sign problem inherent in a full quantum Monte Carlo.

It is important to note that this approach has been explicitly designed to treat the low–temperature regime in which local moments exist, i.e., in which the most probable configurations of $\vec{\xi}^i$ have non–zero amplitude (at least for some sites $i$). We do not address in this paper the problem of local moment formation per se. It is clear that at high temperatures the “free” $\vec{\xi}^i$ fluctuations have variance $\langle \vec{\xi}^i \cdot \vec{\xi}^i \rangle \propto T$, and it is not appropriate to use $S_{\text{eff}}(\xi)$ as a starting point for perturbation theory in this regime. Instead our purpose is to construct an approximation scheme which builds
in the presence of disordered local moments at temperatures satisfying

\[ 4t^2/U \leq T \ll U \]  

(37)

in three dimensions and

\[ T \ll U \]  

(38)

in two dimensions.

It is also important to note that this approximation omits quantum effects associated with “tunneling” of the order parameter fields, i.e., possible \( \tau \)-dependent instantons. As a result the Kondo effect is outside the present description. We restrict our attention here to the implications of a classical (i.e., \( m = 0 \)) order parameter description and do not discuss additional quantum effects.

We next examine the behavior of \( S_{\text{eff}} \) in the large–\( U \) limit, then comment on the action’s relationship to other work in the literature. In the large–\( U \) limit the Hubbard model may be mapped to a quantum spin–\( \frac{1}{2} \) Heisenberg model with near–neighbor antiferromagnetic exchange integral \( J = 4t^2/U \). We show below that in this limit the approximate action \( S_{\text{eff}} \) describes a classical Heisenberg model with exchange integral \( J = 4t^2/U \). This insures that in a two–dimensional system the approximation obeys the Mermin–Wagner Theorem, i.e., infinite–range spin ordering is absent down to \( T = 0 \). However this approach does not include the quantum fluctuations which renormalize the zero–temperature moment and reduce the finite–temperature correlation length. It is essential to include finite–frequency fluctuations in order to address these points. Nevertheless the static action \( S_{\text{eff}} \) achieves the goal of reproducing the exact classical critical behavior within a well–defined zeroth–order approximation.

To demonstrate the mapping to the classical Heisenberg model, consider first the local one–site action \((t = 0)\) in the large–\( U \) limit for \( \langle n \rangle = 1 \):

\[
S_{\text{one-site eff}} = \beta |\xi|^2 - \sum_r \log [1 + e^{-\beta \epsilon_r(\xi)}].
\]  

(39)

In this case there are only two eigenvalues \( \epsilon_r \). To find \( \epsilon_r \), choose the spin quantization axis along the direction of \( \vec{\xi} \). Then the field–dependent term in \( H(\xi) \) is just

\[-\sqrt{U}\xi (c_{i\uparrow}^\dagger c_{i\uparrow} - c_{i\downarrow}^\dagger c_{i\downarrow}) ,
\]  

(40)

with eigenvalues

\[ \epsilon_\alpha = -\sqrt{U}\xi\alpha, \quad \alpha = \pm 1. \]  

(41)

Minimization of the action with respect to \( \xi \) gives

\[ \xi = \sqrt{U} \sum_\alpha \frac{\alpha e^{\beta\alpha\sqrt{U}\xi}}{1 + e^{\beta\alpha\sqrt{U}\xi}} , \]  

(42)

i.e.,

\[ \xi = \frac{1}{2} \sqrt{U} \langle m_z \rangle , \]  

(43)
since
\[ \langle m_z \rangle = \sum_{\alpha = \pm 1} \alpha \frac{1}{1 + e^{-\beta \alpha \sqrt{U} \xi}}. \] (44)

For large \( U \) the solution has
\[ \langle m_z \rangle \to 1 \]
\[ \xi \to \sqrt{U}/2. \] (45)

As expected, the one–site gap is just
\[ \varepsilon_\uparrow - \varepsilon_\downarrow = \frac{1}{2} U - \left( -\frac{1}{2} U \right) = U. \] (46)

Note that this result has been obtained without breaking the rotational invariance of the one–site Hamiltonian, since the direction of \( \vec{\xi} \) is arbitrary, and the Boltzmann weight must be integrated over \( \vec{\xi} \).

Thus to zeroth order in \( t/U \), the half–filled system consists of fluctuating fields \( \vec{\xi}^i \) of fixed length \( \sqrt{U}/2 \) and uncorrelated directions. The first non–zero terms in perturbation theory enter at \( O(t/U)^2 \), and describe the process of one electron hopping to a neighboring site, then back to its starting point. Physically the hopping terms should induce correlations in the field directions at neighboring sites to lower the kinetic energy. Let the field directions at neighboring sites \( i \) and \( j \) be \( \hat{n}^i \) and \( \hat{n}^j \). Suppose also that \( \hat{n}^i \) may be obtained by rotating \( \vec{\xi} \) in a right–handed sense by angle \( \alpha \) about axis \( \vec{\alpha} \perp \vec{\xi} \). Then the eigenstates with spin projection \( \pm \frac{1}{2} \) along \( \hat{n}^i \) can be written
\[ |\hat{n}^i, \uparrow\rangle = \cos \frac{\alpha}{2} |\vec{\xi}, \uparrow\rangle + (-i\alpha_x + \alpha_y) \sin \frac{\alpha}{2} |\vec{\xi}, \downarrow\rangle \]
\[ |\hat{n}^i, \downarrow\rangle = (-i\alpha_x - \alpha_y) \sin \frac{\alpha}{2} |\vec{\xi}, \uparrow\rangle + \cos \frac{\alpha}{2} |\vec{\xi}, \downarrow\rangle, \] (47)
where
\[ \alpha_x^2 + \alpha_y^2 = 1. \] (48)

The one–site solution gives
\[ |\vec{\xi}^i| = \frac{1}{2} \sqrt{U} = \frac{1}{2} \sqrt{U} \langle \hat{n}^i \cdot \vec{m}^i \rangle, \] (49)
so that \( |\hat{n}^i, \uparrow\rangle \) will be occupied and \( |\hat{n}^i, \downarrow\rangle \) will be empty (and higher in energy by \( U \)). Now apply second–order perturbation theory to the electron ground state for the frozen field configuration with direction vectors \( \{\hat{n}^i\} \). The matrix element for hopping from
\[ |\hat{n}^i, \uparrow\rangle \langle \hat{n}^j, \uparrow\rangle \to |\hat{n}^j, \downarrow\rangle \langle \hat{n}^i, \uparrow\rangle \] (50)
is
\[ (-t) \langle \hat{n}^j, \downarrow |\hat{n}^i, \uparrow \rangle = (-t) (-i\theta_x - \theta_y)^* \sin \frac{\theta}{2}, \] (51)
where $\hat{n}_j$ is obtained from $\hat{n}_i$ by a right–handed rotation by $\theta$ about axis $\hat{\theta} \perp \hat{n}_i$. The energy lowering of the ground state due to the virtual hop from $i \to j$ and back is then
\[
\left\{ (-t)(-i\theta_x - \theta_y) \sin(\theta/2) \right\} = -\frac{t^2}{U} \sin^2 \frac{\theta}{2}, \tag{52}
\]
since
\[
\theta_x^2 + \theta_y^2 = 1. \tag{53}
\]
The hopping from $j \to i$ supplies the same energy, so the total perturbation energy lowering in this particular field configuration is
\[
-\frac{2t^2}{U} \sum_{\langle ij \rangle} \sin^2(\theta_{ij}/2) = \frac{t^2}{U} \sum_{\langle ij \rangle} (\cos \theta_{ij} - 1) = \frac{4t^2}{U} \sum_{\langle ij \rangle} \left[ \frac{1}{4} \hat{n}_i \cdot \hat{n}_j - \frac{1}{4} \right]
\]
\[
= \frac{4t^2}{U} \sum_{\langle ij \rangle} \left[ \langle \vec{S}_i \rangle \xi \cdot \langle \vec{S}_j \rangle \xi - \frac{1}{4} \right], \tag{54}
\]
where $\langle \vec{S}_i \rangle \xi$ is the electron spin expectation value in configuration $\{ \xi^i \}$ for $t = 0$. Note finally that the effective action at half–filling reduces to
\[
S_{\text{eff}}(\xi) = \beta \sum_i |\xi^i|^2 - \log \prod_r [1 + e^{-\beta \varepsilon_r(\xi)}]. \tag{55}
\]
In the large–$U$ limit
\[
\prod_r [1 + e^{-\beta \varepsilon_r(\xi)}] \simeq \exp[-\beta E_0(\xi)], \tag{56}
\]
with $E_0$ the perturbed ground state energy, since all other occupancies result in an energy higher by at least $U$. Since $\beta \sum_i |\xi^i|^2$ is a constant in this limit, the part of the action dependent on the fluctuating fields is precisely $\beta H_{\text{eff}}$, with
\[
H_{\text{eff}} = \frac{4t^2}{U} \sum_{\langle ij \rangle} \left( \frac{1}{4} \hat{n}_i \cdot \hat{n}_j - \frac{1}{4} \right), \tag{57}
\]
establishing the mapping to the classical Heisenberg model.

The behavior of the action away from half–filling in the large–$U$ limit is not so easy to deduce, since the Hartree–Fock correction from the static charge interaction is crucial. If one assumes $N_{\text{el}}$ sites are singly occupied and $N_{\text{sites}} - N_{\text{el}}$ sites are empty, the one–site saddle–point equation implies $|\xi^i| = \sqrt{U}/2$ on the singly occupied sites and $|\xi^i| = 0$ on the empty sites. A degeneracy then arises, since the low–lying one–electron states on the singly occupied sites pick up a Hartree–Fock density contribution $(U/2)\langle n^i \rangle = U/2$, while the states on the empty sites have no Hartree–Fock correction. The two sorts of sites then have degenerate low–lying states in the
absence of $t$: The occupied state on each singly occupied site has energy $-\frac{1}{2}U + \frac{1}{2}U = 0$, and the two states on each unoccupied site also have energy 0. As expected, the hopping becomes crucial for determining $\langle n_i \rangle$ and the favored $\vec{\xi}_i$ configurations. Thus in the doped case there are important amplitude, as well as orientation, fluctuations in the S–H field configurations arising from $S_{\text{eff}}$.

We next comment briefly on the relationship of our approximation to other work in the literature. We have argued in Section 1 that perturbation theory in $U$ fails to resum properly at low temperatures in the doped Mott insulator phase due to a fundamental change in the system’s saddle–point structure. Nevertheless a number of authors [7]–[9] have observed that gaps or pseudogaps in the one–electron density of states for the positive–$U$ and negative–$U$ Hubbard models may be obtained within approximations which resemble perturbation theory about a non–interacting ground state. Such approximations have in common the feature that the one–electron self–energy $\Sigma$ may be written in the form

$$\Sigma(k, i\omega_n) = \frac{T}{N_{\text{sites}}} \sum_{Qm} V(Q, i\Omega_m) G_0(k - Q, i(\omega_n - \Omega_m)),$$

(58)

where $V$ is a momentum– and frequency–dependent effective potential and $G_0$ is a bare electron propagator. Crucial points to note are that (i) the electron propagator is left bare; and (ii) higher order perturbation theory in $V$ leads to a deterioration, rather than an improvement, in the approximation for the one–electron density of states. We argue that the reasons for this behavior are as follows: The local moments which underlie the Mott–Hubbard gap generate anomalous diagrams in perturbation theory, i.e., terms in the one–electron self–energy off–diagonal in momentum and spin. At zero temperature and half filling the moments have true long–range staggered order, so that a momentum–space description becomes possible. If the static off–diagonal self–energy is denoted $\Delta_{\vec{Q}}$, with $\vec{Q} = (\pi, \pi)$, then the effective diagonal self–energy becomes

$$\Sigma(k, i\omega_n) = \Delta^2_{\vec{Q}} G_0(k - \vec{Q}),$$

(59)

generating a Hartree–Fock antiferromagnetic gap of $2\Delta_{\vec{Q}}$ in the density of states. In this case, as is well known, $G_0$ enters Eqn. 59 rather than $G$ to avoid double counting. Thus approximations of the form in Eqn. 58 may be viewed as generalizations of Eqn. 59 which “smear” the off–diagonal self–energy $\Delta$ over a range in momentum– and frequency–space [25]. In this sense these approximations are quite different from perturbation theory in $V$, and they do not provide support for the convergence of perturbation theory in the doped Mott insulator. We would argue that such approximations model only roughly the physics of this system [26]. In the doped phase the order parameter field has strong non–Gaussian fluctuations in both amplitude and orientation, and these are coupled to the charge degrees of freedom. Furthermore, as discussed in reference [21], this general approach has difficulties addressing rare large amplitude fluctuations that play an essential role.

We comment also on the relationship of the current approach to the phenomenological spin–fermion (SF) model. In recent years a number of perturbative studies
have been carried out for this model, which describes a system of electrons coupled to a Gaussian–distributed vector spin field $S(Q, i\Omega)$. The microscopic action $S_{\text{eff}}$ differs from $S_{\text{SF}}$ in two crucial ways: (i) $S_{\text{SF}}$ omits coupling to charge degrees of freedom, while $S_{\text{eff}}$ describes a highly nonlinear coupling between spin and charge. The form of this coupling is dictated by the Hubbard interaction itself, and its omission prevents a proper description of the doped Mott insulator phase. (ii) The finite–frequency corrections to the actions differ significantly, since we have introduced only a static S–H field to circumvent the problems associated with an equal–time decoupling. Finally, our point on the non–Gaussian nature of fluctuations in $S_{\text{eff}}$ applies to $S_{\text{SF}}$ as well, i.e., in the interesting parameter regime for this model we expect a conventional perturbative treatment to be impossible due to the formation of local moments.

### 3 Evaluation of electron correlation functions

Electron correlation functions for the action $\overline{S}$ in Eqn. 30 have been calculated using the Metropolis algorithm for statistical sampling of $\xi^i$ configurations. The Monte Carlo algorithm adopted relies on single–site updating and resembles a hybrid of Glauber and Kawasaki dynamics for the Ising or classical Heisenberg models. The algorithm is described more precisely in Section 4.

Electron correlation functions have the same general form as in full quantum Monte Carlo calculations with continuous–valued S–H fields. Let $A(\mathbf{r}, \mathbf{c})$ be an electron observable written in anticommuting c–number notation, and let

$$D\xi = \int \prod_i \left( \frac{\beta}{\pi} \right)^{3/2} d\xi^i_x d\xi^i_y d\xi^i_z .$$

Then

$$\langle A \rangle = \frac{\int D\xi \exp[-\overline{S}_0(\xi)] \int D\mathbf{\bar{c}} D\mathbf{c} A(\mathbf{\bar{c}}, \mathbf{c}) \exp[-\overline{S}_f(\xi, \mathbf{\bar{c}}, \mathbf{c})]}{\int D\xi D\mathbf{\bar{c}} D\mathbf{c} \exp[-\overline{S}_0(\xi)] \exp[-\overline{S}_f(\xi, \mathbf{\bar{c}}, \mathbf{c})]} = \frac{1}{Z} \int D\xi \exp[-\overline{S}_0(\xi)] \left[ \frac{\int D\mathbf{\bar{c}} D\mathbf{c} A(\mathbf{\bar{c}}, \mathbf{c}) \exp[-\overline{S}_f(\xi, \mathbf{\bar{c}}, \mathbf{c})]}{\int D\mathbf{\bar{c}} D\mathbf{c} \exp[-\overline{S}_f(\xi, \mathbf{\bar{c}}, \mathbf{c})]} \right] \overline{Z}_f(\xi) ,$$

where

$$\overline{Z}_f(\xi) = \int D\mathbf{\bar{c}} D\mathbf{c} \exp[-\overline{S}_f(\xi, \mathbf{\bar{c}}, \mathbf{c})] = \prod_r [1 + e^{-\beta\varepsilon_r(\xi)}] ,$$
and the last line in Eqn. 61 follows by multiplying and dividing by $Z_f$ within the integral. The expression in square brackets is just an electron thermal average in the presence of the background $\xi^i$ configuration. Thus finally

$$\langle A \rangle = \frac{1}{Z} \int D\xi \exp[-S_{\text{eff}}(\xi)] \langle A(\tau, c) \rangle_\xi$$

$$= \langle \langle A(\tau, c) \rangle_\xi \rangle,$$  \hspace{1cm} (63)

where

$$S_{\text{eff}}(\xi) = S_0(\xi) - \log Z_f(\xi)$$

$$= S_0(\xi) - \sum_r \log [1 + e^{-\beta \epsilon_r(\xi)}].$$  \hspace{1cm} (64)

The simple form for $S_{\text{eff}}$ means that approximations which incorporate finite–frequency fluctuations, i.e., which generalize $Z_f(\xi)$, may in principle be developed to extend the approach worked out in detail here (see Section 6).

We derive below the form of several one– and two–body electron correlation functions $\langle A(\tau, c) \rangle_\xi$ in the presence of the background fields. As stated previously,

$$\langle n^i \rangle_\xi = \sum_\alpha G_{\alpha\alpha}(ii; \tau = 0^-)$$

$$= \sum_r f(\epsilon_r) |\langle r|\alpha \rangle|^2,$$  \hspace{1cm} (65)

where

$$G_{\alpha\alpha'}(ij; \tau) = -\langle c^{i\alpha}(\tau)|c^{j\alpha'}(0)\rangle_\xi$$

in terms of anticommuting c–numbers; and the $|r\rangle$ are eigenstates of the spin–dependent Hamiltonian $H(\xi)$ in Eqn. 33. Likewise, the spin polarization at site $i$ is

$$\langle \vec{m}^i \rangle_\xi = \sum_{\alpha\alpha'} \langle \vec{c}^{i\alpha} | \vec{\sigma}_{\alpha\alpha'} | c^{i\alpha'} \rangle_\xi$$

$$= \sum_{\alpha\alpha'} \vec{\sigma}_{\alpha\alpha'} G_{\alpha'\alpha}(ii; \tau = 0^-)$$

$$= \sum_{r\alpha\alpha'} f(\epsilon_r) \vec{\sigma}_{\alpha\alpha'} \langle r|\alpha \rangle \langle \alpha'|r \rangle,$$  \hspace{1cm} (67)

in terms of the $S_z$–basis states $|\alpha \rangle$. Writing out the vector components explicitly gives

$$\langle m^i_x \rangle_\xi = \sum_r f(\epsilon_r) \left[ \langle i \downarrow |r \rangle \langle r|i \uparrow \rangle + \langle i \uparrow |r \rangle \langle r|i \downarrow \rangle \right]$$

$$\langle m^i_y \rangle_\xi = \sum_r f(\epsilon_r) \left[ -i \langle i \downarrow |r \rangle \langle r|i \uparrow \rangle + i \langle i \uparrow |r \rangle \langle r|i \downarrow \rangle \right]$$

$$\langle m^i_z \rangle_\xi = \sum_r f(\epsilon_r) \left[ |\langle i \uparrow |r \rangle|^2 - |\langle i \downarrow |r \rangle|^2 \right].$$  \hspace{1cm} (68)
Note that these last results generalize to give the one–body propagator

\[ G_{i\alpha,j\beta}(i\omega_n)\xi = \int_0^\beta d\tau e^{i\omega_n\tau} \left[ -\langle e^{i\alpha(\tau)}\sigma^j\beta(0)\rangle\xi \right] = -\beta \langle e^{i\alpha\tau}\sigma^j\beta \rangle\xi \]

\[ = \sum_r \frac{\langle i\alpha|r\rangle \langle r|j\beta \rangle}{i\omega_n - \varepsilon_r} \] \hspace{1cm} (69)

The real–axis spectral density may be calculated directly by analytic continuation before the field averaging is performed. Thus the one–particle spectral density for spin \( \alpha \) at site \( i \) after field–averaging is

\[ N_{i\alpha}(\omega) = -\frac{1}{\pi} \left\langle \text{Im} \ G_{\alpha\alpha}(ii; \omega + i0^+)\xi \right\rangle \]

\[ = \left\langle \sum_r |\langle i\alpha|r\rangle|^2 \delta(\omega - \varepsilon_r) \right\rangle . \] \hspace{1cm} (70)

The total one–particle spectral density for spin \( \alpha \) is

\[ N_{\alpha}(\omega) = \sum_i N_{i\alpha}(\omega) . \] \hspace{1cm} (71)

(Note that in a properly equilibrated calculation translational and spin–rotational invariance are restored by field–averaging, and the quantity \( N_{i\alpha} \) is site– and spin–independent.) The momentum–resolved spectral density \( A_{k\alpha}(\omega) \) is only slightly more difficult to calculate. Note again that translational invariance is only restored by field–averaging, so that the propagator in a single field configuration is not diagonal in momentum. After averaging we have

\[ A_{k\alpha}(\omega) = \left\langle \sum_r \delta(\omega - \varepsilon_r) \cdot \frac{1}{N_{\text{sites}}} \sum_{ij} e^{-ik \cdot (R_i - R_j)} \langle i\alpha|r\rangle \langle r|j\alpha \rangle \right\rangle \] \hspace{1cm} (72)

All the spectral densities may be calculated conveniently by histogram binning, i.e., by incrementing a bin centered on frequency \( \omega_i \) whenever an eigenvalue \( \varepsilon_r \) falls in the range \([\omega_i - (1/2)\Delta\omega, \omega_i + (1/2)\Delta\omega]\). In this way spectral densities may be obtained which integrate exactly to unity within machine precision.

In some cases it may be desirable to compare imaginary–time propagators \( G_{k\alpha}(\tau) \) with the results from a full quantum Monte Carlo simulation. The necessary expressions within the present approach are

\[ G_{k\alpha}(\tau) = \begin{cases} 
-\sum_r e^{-\varepsilon_r\tau} \left[ 1 - f(\varepsilon_r) \right] F^r_{k\alpha}, & \tau > 0 \\
\sum_r e^{-\varepsilon_r\tau} f(\varepsilon_r) F^r_{k\alpha}, & \tau < 0 
\end{cases} \] \hspace{1cm} (73)

where

\[ F^r_{k\alpha} = \frac{1}{N_{\text{sites}}} \sum_{ij} e^{-ik \cdot (R_i - R_j)} \langle i\alpha|r\rangle \langle r|j\alpha \rangle . \] \hspace{1cm} (74)
A quantity of particular interest in the local moment regime is the average double occupancy

$$\langle D \rangle = \frac{1}{N_{\text{sites}}} \sum_i \langle D_i^{(i)} \rangle, \quad (75)$$

where

$$\langle D_i^{(i)} \rangle = \langle n_i^{(i)} n_i^{(i)} \rangle. \quad (76)$$

In a general \( \xi^i \) configuration with broken spin–rotational invariance the appropriate expression for \( \langle D_i^{(i)} \rangle \) is not \( \langle n_i^{(i)} \rangle \langle n_i^{(i)} \rangle \). Instead

$$\langle D_i^{(i)} \rangle = \lim_{\tau \to \tau'} \langle \sigma_i^{(i)} c_i^{(i)}(\tau') \sigma_i^{(i)} c_i^{(i)}(\tau') \rangle_{\xi} = \langle n_i^{(i)} \rangle \langle n_i^{(i)} \rangle + \langle c_i^{(i)} \sigma_i^{(i)} \rangle \langle \sigma_i^{(i)} c_i^{(i)} \rangle_{\xi}. \quad (77)$$

Note

$$\langle \sigma_i^{(i)} c_i^{(i)} \rangle_{\xi} = \frac{1}{2} [\langle m_i^z \rangle_{\xi} + i \langle m_i^y \rangle_{\xi}],$$
$$\langle c_i^{(i)} \sigma_i^{(i)} \rangle_{\xi} = -\frac{i}{2} [\langle m_i^z \rangle_{\xi} - i \langle m_i^y \rangle_{\xi}], \quad (78)$$

while

$$\langle n_i^{(i)} \rangle_{\xi} = \frac{1}{2} [\langle n_i^{(i)} \rangle_{\xi} + \langle m_i^z \rangle_{\xi}],$$
$$\langle n_i^{(i)} \rangle_{\xi} = \frac{1}{2} [\langle n_i^{(i)} \rangle_{\xi} - \langle m_i^z \rangle_{\xi}]. \quad (79)$$

Thus

$$\langle D_i^{(i)} \rangle_{\xi} = \frac{1}{4} [\langle n_i^{(i)} \rangle_{\xi}^2 - \langle \sigma_i^{(i)} \rangle_{\xi} \cdot \langle \bar{m}_i^{(i)} \rangle_{\xi}]. \quad (80)$$

The double occupancy assumes an explicitly spin–rotation–invariant form as required.

The expression in Eqn. (80) should in principle be supplemented by zero– and finite–frequency RPA corrections to insure that Eqn. (77) reproduces the \( \tau \to \tau' \) limit of the general two–body correlation function. (As noted below in the discussion of response functions, RPA corrections appear at zero frequency because the charge interaction is being treated within Hartree–Fock. There is no zero–frequency RPA in the spin channel, since that portion of the interaction is being treated exactly.) RPA corrections in equal–time expectation values \( \langle n_{\alpha}(\tau) n_{\alpha'}(\tau') \rangle \) are actually problematic in any perturbation theory for the following reason: The Pauli Principle implies an exact identity

$$\langle n_{\alpha}(\tau) n_{\alpha'}(\tau) \rangle = \langle n_{\beta} \rangle. \quad (81)$$

In perturbation theory, this identity can only be preserved exactly in approximations with a crossing–symmetric two–body vertex. Such a vertex appears in order–by–order perturbation theory (and in parquet theory), but not in a standard RPA, whether about the unperturbed vacuum or about broken–symmetry states as in the present case. The RPA can be augmented to make it crossing–symmetric by incorporating the missing contributions in the crossed channel (see Figure 3), but the result is no longer conserving in the Baym–Kadanoff sense. The RPA corrections to the double
occupancy are in any event expected to be small in the present case. Since they are also problematic, we omit them from the calculation of \( \langle D \rangle \) reported here.

We next consider the static spin and charge susceptibilities \( \chi_s(Q) \) and \( \chi_c(Q) \). As mentioned above, one expects the appearance of RPA corrections in the static charge response, since the charge interaction is being treated by “slave” Hartree–Fock, but naively one might expect no corrections in the spin response. This is not correct: An average must be performed over the symmetry–breaking field \( \vec{\xi}^i \), and in the presence of \( \vec{\xi}^i \) spin and charge excitations are mixed. For this reason the repulsive charge interaction makes its presence felt weakly in the spin channel, as well as in the charge channel.

The static spin response function takes the form

\[
\chi_{ij}^{\mu\nu} \equiv \partial \left. \langle \langle m^i_\mu \rangle \rangle / \partial h^j_\nu \right|_{h=0},
\]

(82)

where the assumed local coupling to the external field \( \vec{h}^j \) is

\[
\Delta H = -\vec{h}^j \cdot \sum_{\alpha\alpha'} c^\dagger_{j\alpha} \sigma_{\alpha\alpha'} c_{j\alpha'}.
\]

(83)

Temporarily neglecting RPA corrections, the field derivative yields

\[
\chi_{ij}^{\mu\nu} = -\frac{1}{T} \left( \langle \langle m^i_\mu \rangle \rangle \langle \langle m^j_\nu \rangle \rangle - \langle \langle m^i_\mu \rangle \rangle \langle \langle m^j_\nu \rangle \rangle \right) + \frac{1}{T} \left\langle \sum_n \sum_{\alpha\alpha'} \sum_{\beta\beta'} G_{\beta\alpha} (ij; i\omega_n) \sigma_{\alpha\alpha'} \sigma_{\beta\beta'} (ij; i\omega_n) \right\rangle.
\]

(84)

The first term on the right–hand–side vanishes for zero applied field (since the system has no spontaneous magnetization at finite temperature), and the second term (see Figure 4) reduces to

\[
\chi_{ij}^{\mu\nu} = \frac{1}{T} \left( \langle \langle m^i_\mu \rangle \rangle \langle \langle m^j_\nu \rangle \rangle - \langle \langle m^i_\mu \rangle \rangle \langle \langle m^j_\nu \rangle \rangle \right) + \left( -T \sum_n \sum_{\alpha\alpha'} \sum_{\beta\beta'} G_{\beta\alpha} (ij; i\omega_n) \sigma_{\alpha\alpha'} \sigma_{\beta\beta'} \right),
\]

(85)

i.e., formally an “anomalous” and a “normal” contribution. The anomalous contribution may be evaluated using previous expressions for the site spin polarizations, while the normal term may be written as the configurational average of

\[
\sum_{\alpha\alpha', \beta\beta'} M^{ij}_{\alpha\alpha', \beta\beta'} (i\Omega = 0) \sigma_{\alpha\alpha'} \sigma_{\beta\beta'}.
\]

(86)

where

\[
M^{ij}_{\alpha_1\alpha_2, \beta_1\beta_2} (i\Omega) \equiv -\sum_{r,s} \langle j\beta_1 | r \rangle \langle r | i\alpha_1 \rangle \langle i\alpha_2 | s \rangle \langle s | j\beta_2 \rangle \frac{f(\varepsilon_r) - f(\varepsilon_s)}{\varepsilon_r + i\Omega - \varepsilon_s}.
\]

(87)

(Note that for \( \varepsilon_r = \varepsilon_s \), the ratio involving the Fermi functions must be replaced by \( f'(\varepsilon_r) \delta_{\Omega 0} \). )
The static charge response function is
\[ \chi^{ij} \equiv \frac{\partial \langle \langle n^i \rangle \rangle_{\xi}}{\partial \mu^j} \bigg|_{\mu=0}, \tag{88} \]
where in this case the assumed coupling to the external field is
\[ \Delta H = -\mu^j \sum_{\alpha} c_{j\alpha}^\dagger c_{j\alpha}. \tag{89} \]

In complete analogy with the spin response calculation the result before the inclusion of RPA corrections is
\[ \chi^{ij} = \frac{1}{T} \left[ \langle \langle n^i \rangle \xi \langle n^j \rangle \xi \rangle - \langle n \rangle^2 \right] \]
\[ + \sum_{\alpha\alpha',\beta\beta'} \langle M^{ij}_{\alpha\alpha',\beta\beta'}(i\Omega = 0) \xi \rangle \delta_{\alpha\alpha'} \delta_{\beta\beta'}, \tag{90} \]
with the normal “bubble” \( M \) defined as in Eqn. 87.

As emphasized above, RPA corrections necessarily appear when an interaction is treated perturbatively by Hartree–Fock. In the present case, where spin and charge excitations mix before the configurational average is performed, RPA charge vertex corrections appear in both the static charge and spin response functions.

The calculation of RPA corrections for finite–frequency response functions is trickier than in conventional perturbation theory because the zero–frequency spin vertices have been explicitly removed from the theory. This affects response functions at \( i\Omega \neq 0 \) by partially removing vertices which carry zero frequency in a crossed particle–hole channel. The analytic continuation to real energies is also complicated by this feature of the theory. We defer discussion of spin and charge response at finite frequency and concentrate in the present paper on RPA corrections to the static susceptibilities.

The repulsive RPA charge vertex produces a geometric series of corrections as in conventional perturbation theory. Due to the lack of symmetry in individual configurations, the series can only be summed in matrix form. Writing
\[ V^{ij}_{\alpha_1\alpha_2,\beta_1\beta_2} = \frac{1}{2} U \delta_{ij} \delta_{\alpha_1\alpha_2} \delta_{\beta_1\beta_2}, \tag{91} \]
the complete RPA–corrected expressions for the spin and charge susceptibilities are given by
\[ \chi^{ij}_{\mu\nu} = \frac{1}{T} \left[ \langle \langle m^i_{\mu} \rangle_n \langle m^j_{\nu} \rangle_n \rangle + \sum_{\alpha\alpha',\beta\beta'} \langle \left[ M(1 + VM)^{-1} \right]^{ij}_{\alpha\alpha',\beta\beta'}(i\Omega = 0) \xi \rangle \sigma^\mu_{\alpha\alpha'} \sigma^\nu_{\beta\beta'}, \tag{92} \right. \]

and
\[ \chi^{ij} = \frac{1}{T} \left[ \langle \langle n^i \rangle \xi \langle n^j \rangle \xi \rangle - \langle n \rangle^2 \right] \]
\[ + \sum_{\alpha\alpha',\beta\beta'} \langle \left[ M(1 + VM)^{-1} \right]^{ij}_{\alpha\alpha',\beta\beta'}(i\Omega = 0) \xi \rangle \delta_{\alpha\alpha'} \delta_{\beta\beta'}. \tag{93} \]
Finally the momentum–resolved spin susceptibility takes the form

$$\chi_{\mu\nu}(Q) = \frac{1}{N_{\text{sites}}} \sum_{ij} e^{iQ \cdot (R_i - R_j)} \chi_{ij}^\mu \chi_{ij}^\nu, \quad (94)$$

and similarly for the charge susceptibility. (Measurements of the RPA–corrected susceptibilities require the inversion of small matrices, but the effect on overall calculational efficiency is negligible.)

4 Description of the Monte Carlo algorithm

The effective action in Eqn. 64 has been simulated using the Metropolis algorithm. In comparison with a classical Heisenberg spin model, the present theory has several complications: (i) The theory has three degrees of freedom (orientation on the unit sphere and amplitude) at each site, rather than two. (ii) Local field updates induce global changes in the action through the Fermi partition function $Z_f(\xi)$. (iii) A Hartree–Fock convergence step is necessary after each spin field update to keep the “slave” charge fields $\langle n^i \rangle_\xi$ on the saddle point. (iv) Single–site updating (i.e., Glauber dynamics) is insufficient to achieve efficient equilibration for $\langle n \rangle \neq 1$. An analog of Kawasaki dynamics, or spin swapping, is required, since the doping $1 - \langle n \rangle$ plays a role similar to a conserved order parameter.

We consider each complication in turn. (i) The natural physical interpretation of field fluctuations in terms of amplitude and orientation suggests an optimal representation for the functional integral over field configurations. At half–filling it is expected that the only important fluctuations for $T \to 0$ correspond to magnons, i.e., slow modulations of the field orientation for fixed amplitude. A Cartesian representation of the fields $(\xi^i_x, \xi^i_y, \xi^i_z)$ with independent component updates leads to a small acceptance ratio in the low–temperature limit. Therefore we write

$$\int d\xi_x^i d\xi_y^i d\xi_z^i = \int_0^\infty (r^i)^2 dr^i \int_{-1}^1 d(cos \theta^i) \int_0^{2\pi} d\phi^i, \quad (95)$$

choosing as independent variables $r^i$, $x^i \equiv \cos \theta^i$, and $\phi^i$. Variations in the measure $(r^i)^2$ at each site are incorporated into the Metropolis updating factor, and moves are restricted, in a way consistent with detailed balance, to lead to $r^i > 0$. Proposed changes to $r^i$ are restricted to a maximum scale $\Delta r$, while large–scale changes are permitted in $x^i$ and $\phi^i$.

(ii) For the initial Monte Carlo calculations reported here we have simply diagonalized the effective Hamiltonian matrix $H(\xi)$, which has row dimension $2N_{\text{sites}}$, for each proposed $\vec{\xi}$ configuration. The time for a single site update thus grows as the cube of the system size, and the time for a lattice sweep as the fourth power of the system size. We believe that a hybrid molecular–dynamics/Monte–Carlo algorithm
can be developed to significantly reduce the time needed for the simulation of large lattices [31].

(iii) The Hartree–Fock treatment of the static charge interaction is an integral component of the present approach. More sophisticated treatments of fluctuations would also in principle involve a self–consistent calculation in the presence of symmetry–breaking background fields. For the parameter sets studied in the present paper, the Hartree–Fock iteration loop generally converges in three to four steps. Since each step requires a matrix rediagonalization, overall calculational time scales with the average number of Hartree–Fock iterations.

(iv) At half–filling the Hartree–Fock charge–field convergence becomes trivial, and \( \langle n^i \rangle \) remains equal to unity at all sites in all configurations. This just reflects the particle–hole symmetry of the model for this special parameter set. Away from half–filling the situation is quite different. Typical configurations contain a few sites with small fields, while the majority of sites have fields with amplitudes close to the half–filled value. Conventional single–spin updating tends to leave “holes” trapped at isolated locations, since moving a hole requires passing through high–energy intermediate configurations. In this sense the number of hole \( 1 - \langle n \rangle \) functions like a conserved order parameter, preventing the equilibration of the system by Glauber dynamics. To combat this effect we have introduced a second type of updating move, viz., a swap of the spin fields \( \vec{\xi} \) at two sites chosen at random. When the spin fields are swapped, the “slave” charge fields are dragged along, and the system equilibrates to a uniform set of site occupancies \( \langle \langle n^i \rangle \rangle \), even though the hole distribution in individual configurations is highly non–uniform.

5 Numerical results for a small Hubbard lattice

The results for 4 \( \times \) 4 periodic lattices reported below were obtained on an IBM PowerPC work station and a Sun–3000 server. For all runs reported here, a total of 100 Monte Carlo warmup sweeps and 5000 sampling sweeps were carried out. Runs on 8 \( \times \) 8 and 10 \( \times \) 10 lattices are now in progress on a Sun–10000 work station array at the San Diego Supercomputer Center.

The total density of states for spin \( \alpha \), \( N_\alpha(\omega) \), is plotted in Figure 5 for \( U/t = 4 \) and in Figure 6 for \( U/t = 8 \), both at temperature \( T/t = 0.125 \). The chemical potential \( \mu/t \) is lowered from \( U/2 \) (half–filling) as holes are doped into the insulating state. The mean site occupancy \( \langle n \rangle \) and double occupancy \( \langle D \rangle \) are summarized in Table 1. Note that the double occupancy at half–filling is reduced by factors of order two and six from the value 0.25 for a non–interacting system. A prominent Mott–Hubbard gap, or pseudogap, appears in the density of states for both parameter sets at half–filling (Figures 5a and 6a). The remnants of the discrete quantum energy levels in the non–interacting system remain visible. Note again that these systems are not magnetically ordered: The spin–up and spin–down densities of states are identical.
within statistical sampling errors, and the spin susceptibility is isotropic, as discussed below.

As the chemical potential is pulled below \( \mu = U/2 \), the site occupancy changes slowly at first, particularly for the large charge gap which appears when \( U/t = 8 \) (Figures 6b–c). This is just what one would expect for rigid–band doping in a semiconductor, and such behavior has been observed in previous Lanczos [32, 33] and quantum Monte Carlo [34] studies of the Hubbard model on small lattices [35]. Note that the rigid–band picture begins to break down as soon as the site occupancy drops appreciably below unity (Figure 5b). In the doped system with \( U/t = 4 \) and \( \mu/t = 1.2 \), spectral weight has been drawn from the lower edge of the upper Hubbard band into the gap. Due to this transfer of weight, the gap feature rapidly collapses with doping, though remnants remain for a wide range of fillings (Figures 5c–d). By the time \( \mu/t \) reaches 0.4 for \( U/t = 4 \), the shape of the non–interacting band has begun to re–emerge, though levels are still significantly broadened by the fluctuating spin background.

This broadening is especially evident in the evolution of the k–resolved spectral density for points near the Fermi surface. Recall that a special symmetry of the \( 4 \times 4 \) lattice induces an equivalence between the generally distinct k–points \((\pi, 0)\) and \((\pi/2, \pi/2)\). This means all points on the half–filled Fermi surface have the same \( A_{k\alpha}(\omega) \) for the small systems discussed here. To contrast the behavior of points near and far from the Fermi surface, we plot \( A_{k\alpha}(\omega) \) for \( k = (\pi, 0) \) and \( k = (\pi, \pi) \) at \( U/t = 4 \) in Figures 7 and 8. While the \((\pi, \pi)\) point at the top of the band (Figure 8) has a sharp quasiparticle–like spectral density whose profile changes only slightly with doping, the \((\pi, 0)\) point behaves quite differently. At half–filling \( A_{k\alpha} \) for this point is symmetrically split between the upper and lower Hubbard band edges, just as one would expect in an antiferromagnetic Hartree–Fock solution [1]. Away from half–filling, the spectral density remains exceptionally broad, reflecting the continued presence of strong short–range antiferromagnetic correlations between the fluctuating spins in the doped system. As noted above in the discussion of \( N(\omega) \), remnants of the half–filled gap remain for a wide range of fillings. The spectral broadening decreases for fillings far from unity, consistent with the restoration of the non–interacting band profile (and presumably the recovery of Fermi liquid behavior).

A broadening of the spectral density is also present in perturbative studies, including self–consistent–field methods such as FLEX [3]; however, the details of the broadening mechanism are quite different in the present case. FLEX and phenomenological spin–fluctuation models [29, 36] assume a small–amplitude scattering mechanism which may be treated by perturbation theory about a non–interacting (i.e., Fermi liquid) background. In contrast the present approach treats scattering by large–amplitude background distortions, with highly non–Gaussian static fluctuations in both amplitude and orientation; these distortions evolve smoothly into the ordered antiferromagnetic background at half filling and zero temperature.

The behavior of the spectral density at the \((\pi, 0)\) point for \( U/t = 8 \) is illustrated in Figure 9. As expected, the spectral weight is split symmetrically at half–filling, and
the two peaks are separated by an energy of order $U$. In contrast with the $U/t = 4$ result, the weight is distributed broadly throughout the upper and lower Hubbard bands. Signs of a more narrow coherent feature in the doped lower band are present for $\mu/t = 1.8$ (Figure 9c).

The momentum dependence of the static charge and spin susceptibilities is plotted in Figures 10 and 11 for $U/t = 4$ and 8 at temperature $T/t = 0.125$. Note that the uniform charge susceptibility (or compressibility) is exponentially small at half–filling, as expected for a system with a charge gap. In addition the compressibility increases very rapidly with doping; Note particularly the increase for $U/t = 8$ (Figure 11a). For general fillings $\chi_c(Q)$ is relatively small (note the difference in scales for the charge and spin susceptibility) and structureless at this temperature. This is expected in such a small system. Possible manifestations of charge ordering within the fluctuating spin background may become apparent, however, in larger systems.

In contrast the spin susceptibility is large and strongly peaked at the antiferromagnetic wave vector $(\pi, \pi)$. The peak is expected to move off $(\pi, \pi)$ for doped systems on larger lattices. For the parameter sets illustrated here, the spin susceptibility is dominated by the contributions of the “anomalous” term

$$\frac{1}{N_{\text{sites}}} \sum_{ij} e^{iQ \cdot (R_i - R_j)} \left\langle \frac{\langle m^i_{\mu} \xi \rangle \langle m^j_{\nu} \xi \rangle}{T} \right\rangle. \quad (96)$$

The $\mu\nu = zz$ component of $\chi_s$ is actually plotted in Figures 10 and 11. For 5000 lattice sweeps the agreement between the $xx$, $yy$, and $zz$ components of the $(\pi, \pi)$ spin susceptibility is at the level of the statistical error bars, i.e., a few percent. (The agreement can be arbitrarily improved by increasing the Monte Carlo sampling time.)

6 Extension to higher order Baym–Kadanoff approximations

The present approach consists of simulation of the action for a set of local static fields coupled to electron spin degrees of freedom. When the action is constrained to be at its temperature–dependent global saddle point (if such a point indeed exists in the most general case), these static fields are determined by inhomogeneous Hartree–Fock equations and reduce to the anomalous fields of conventional diagrammatic perturbation theory. Just as Hartree–Fock theory with an anomalous self–energy may be extended using the Baym–Kadanoff prescription [24], there is no formal barrier preventing such an extension in the present case. The computational cost of carrying out self–consistent–field (SCF) perturbation theory in a broken–symmetry background is quite large, however, since total momentum and spin are no longer good quantum numbers. In this section we sketch out the steps necessary for a generalized approach and note several of the technical pitfalls which must be studied and overcome.
The form for the SCF action must be determined separately for each configuration of the $\xi^i$ fields. In full analogy with Baym–Kadanoff theory for a uniform system, the action takes the form

$$S^{SCF}(\xi) = \beta \sum_i |\xi^i|^2 - \text{Tr} \log (-G^{SCF}_{\Delta})^{-1} + \beta \mathcal{F},$$  \hspace{1cm} (97)$$

where

$$\mathcal{F}(\xi) = -\text{Tr} (\Sigma G^{SCF}) + \Phi$$  \hspace{1cm} (98)$$

and

$$\frac{\delta \Phi}{\delta G^{SCF}_{\sigma\sigma'}(xx')} = \Sigma_{\sigma'\sigma}(x'x).$$  \hspace{1cm} (99)$$

In these formal expressions $G^{SCF}_{\Delta}$ is the discrete–time propagator (retained to insure a proper high–frequency regularization of the Tr log term);

$$x \equiv (r^i, \tau),$$  \hspace{1cm} (100)$$

and $\Phi$ is the SCF generating functional (e.g., a sum of ring and ladder diagrams in FLEX).

Since the SCF action may be interpreted as $\beta \mathcal{F}^{SCF}$, with $\mathcal{F}^{SCF}$ a well–behaved free energy, the statistical weighting factor $\exp(-S^{SCF})$ is positive definite. This is in sharp contrast to the behavior in imaginary–time quantum Monte Carlo simulations, where the weighting factor can be positive or negative with nearly equal probability.

What is not so clear is the nature of approximations which insure the stability of $S^{SCF}$, particularly for exponentially rare field configurations. The interaction which enters $S^{SCF}$ is not the original Hubbard interaction, since the zero–frequency spin components have been removed for special treatment. This means that there are no obvious zero–frequency instabilities left to appear in $S^{SCF}$. Behavior at finite frequencies must also be addressed, however, and we are not prepared to comment on the stability of general Baym–Kadanoff approximations (and in particular FLEX) in the present paper.

As an example of the Baym–Kadanoff prescription in practice, note that when the static charge interaction is treated within Hartree–Fock

$$\Sigma_{\sigma\sigma'}(xx') = \frac{1}{2}U \langle n^i \rangle_\xi \delta_{ii'} \delta_{\tau \tau'} \delta_{\sigma \sigma'}. $$  \hspace{1cm} (101)$$

The appropriate generating functional is

$$\Phi = \frac{1}{4}U \sum_i \langle n^i \rangle_\xi^2.$$  \hspace{1cm} (102)$$

Furthermore

$$\text{Tr} (\Sigma G^{SCF}) = 2 \Phi$$  \hspace{1cm} (103)$$

and so

$$\mathcal{F} = -\Phi = -\frac{1}{4}U \sum_i \langle n^i \rangle_\xi^2.$$  \hspace{1cm} (104)$$
Note that this form for the Hartree–Fock “constant” in the action is exactly that which has appeared previously in Eqn. [31].

7 Some speculations and conclusions

We believe the present Hubbard model analysis, based on Monte Carlo simulation of a classically disordered local spin field, incorporates several desirable features which have eluded previous perturbative studies. Most important the present theory has classical critical behavior at half–filling and describes the formation of a Mott–Hubbard gap (or pseudogap) in a system with a finite spin correlation length. In addition the spectral densities for the doped systems have the features suggested by exact methods.

The present static field analysis can be extended to significantly larger systems. Since the computations involve Monte Carlo field sampling and have reasonably small memory requirements, it would be natural to carry out studies on multiple processors with different random seeds, then to merge the equilibrated results from numerous short runs.

It is almost unavoidable to speculate on the implications for charge density wave or stripe formation [37, 38] and d–wave singlet pairing in the cuprate superconductors. Since the present approach reduces to standard inhomogeneous Hartree–Fock for $T \rightarrow 0$, Hartree–Fock results previously obtained for stripe formation should re–emerge [2]. By allowing sampling of configurations removed from the zero–temperature saddle point in a well–defined way, the present approach provides a framework to describe the destruction of striped order by thermal fluctuations.

To study potential d–wave superconductivity it seems essential to incorporate the exchange of low–frequency spin fluctuations about the disordered background configurations. The low–energy fluctuations which become magnons in the directions transverse to an ordered spin state (i.e., the Goldstone modes of the order parameter field) must evolve into a broadened spectrum of fluctuations in the important disordered configurations. If low–frequency spin fluctuations are important, the pair order parameter should exhibit retardation effects, in contrast with the spin order parameter. In addition the disordered background has important implications for the onset of pairing. Presumably the pair field appears initially with a highly non–uniform distribution in a small subset of $\vec{\xi}$ configurations. Such behavior would imply superconducting precursor effects in the density of states well above the transition temperature for global phase coherence. The effects would be more akin to the behavior of a system of superconducting grains with variable grain size than to conventional Kosterlitz–Thouless phase fluctuations in a clean two–dimensional superconductor.

In any case the scenario described above is at this stage purely speculative. The next steps in the development of the present approach consist of (i) studies of larger systems; (ii) analysis of the spin and charge response at finite frequencies, with particular care given to the treatment of potential instabilities in rare field configurations.
(see Section 6); and (iii) analysis of pairing eigenvalues and eigenvectors from exchange of fluctuations in sets of non-uniform configurations.

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It is possible to provide a heuristic derivation of a one-electron self-energy with the general form in Eqn. 58 starting from the full theory for $S_{\text{eff}}$ in Section 2. The steps are as follows: (i) Write down the expression for the one-electron propagator dictated by Eqn. 61. (ii) Expand the expression for $G_{i\alpha,j\beta}(i\omega_n)\xi$ within the $\xi^i$ integral as a power series in $\xi^i \cdot \vec{\sigma}$, noting that the odd-order terms integrate to zero. (iii) Resum the series within the integral as $[G_0^{-1}(i\omega_n) - \Sigma(i\omega_n)\xi]^{-1}$, where $\Sigma(i\omega_n)\xi$ takes the form of a self-energy second-order in $\xi^i$. (iv) Approximate the resulting field integral as $[G_0^{-1}(i\omega_n) - \langle \Sigma(i\omega_n)\xi\rangle]^{-1}$, i.e., average the second-order self-energy, rather than the propagator. The field-averaged self-energy assumes exactly the form of Eqn. 58 with $V$ proportional to the full static spin susceptibility of the system. The electron propagator which appears in the self-energy is bare for the reason discussed in the text. Step (iv) is of course not justifiable, since the action is strongly non-Gaussian, but it provides the phenomenological link between some previous theories and the current work.

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Table 1. Mean occupancy $\langle n \rangle$ and double occupancy $\langle D \rangle$ for parameter sets at $T/t = 0.125$. Statistical errors are in the last digit.

| $U/t$ | $\mu/t$ | $\langle n \rangle$ | $\langle D \rangle$ |
|-------|---------|---------------------|---------------------|
| 4.0   | 2.0     | 1.00                | 0.118               |
| 4.0   | 1.2     | 0.93                | 0.105               |
| 4.0   | 1.0     | 0.88                | 0.095               |
| 4.0   | 0.8     | 0.83                | 0.086               |
| 4.0   | 0.6     | 0.77                | 0.078               |
| 4.0   | 0.4     | 0.72                | 0.071               |
| 8.0   | 4.0     | 1.00                | 0.037               |
| 8.0   | 2.4     | 0.99                | 0.037               |
| 8.0   | 1.8     | 0.95                | 0.033               |
Figure 1: Diagrammatic representation of the Hubbard interaction vertex.
Figure 2: Rewriting of the Hubbard interaction vertex in the two crossed particle–hole channels. (a) Transverse spin channel. (b) Longitudinal spin and charge channel.
Figure 3: Example of reducible and irreducible particle–hole vertex diagrams related by crossing symmetry. The third–order reducible vertex appears in an RPA summation. It must be augmented by the irreducible particle–hole vertex shown in order to preserve the Pauli Principle identity in Eqn. [81].
Figure 4: Contributions to the static spin response function. (a) “Anomalous” diagram. (b) “Normal” diagram.
Figure 5: Total density of states for spin $\alpha$, $N_\alpha(\omega)$. The interaction strength is $U/t = 4$, and the temperature is fixed at $T/t = 0.125$. Results are shown for four different chemical potentials. See Table 1 for the mean site occupancy and double occupancy values. Note that in the absence of statistical sampling error $N_\uparrow(\omega) = N_\downarrow(\omega)$. Therefore the measured difference in these two quantities provides a point-by-point error estimate. The vertical dashed line at $\omega = 0$ is drawn to emphasize the position of the chemical potential. (a) $\mu/t = 2.0$. (b) $\mu/t = 1.2$. (c) $\mu/t = 0.8$. (d) $\mu/t = 0.4$. 
Figure 6: Total density of states for spin \( \alpha \), \( N_\alpha(\omega) \). The interaction strength is \( U/t = 8 \), and the temperature is fixed at \( T/t = 0.125 \), as in Figure 5. See Table 1 for the mean site occupancy and double occupancy values. (a) \( \mu/t = 4.0 \). (b) \( \mu/t = 2.4 \). (c) \( \mu/t = 1.8 \).
Figure 7: Momentum–resolved spectral density $A_{k\alpha}(\omega)$. The model parameters are $U/t = 4$ and $T/t = 0.125$, as in Figure 5. The momentum point chosen is $k = (\pi, 0)$. (a) $\mu/t = 2.0$. (b) $\mu/t = 0.8$. (c) $\mu/t = 0.4$. 

![Graphs](image-url)
Figure 8: Momentum–resolved spectral density $A_{k\alpha}(\omega)$. The model parameters are as in Figure 5 and 7. The momentum point chosen is $k = (\pi, \pi)$. (a) $\mu/t = 2.0$. (b) $\mu/t = 0.4$. 
Figure 9: Momentum–resolved spectral density $A_{ka}(\omega)$. The model parameters are $U/t = 8$ and $T/t = 0.125$, as in Figure 6. The momentum point chosen is $k = (\pi, 0)$. (a) $\mu/t = 4.0$. (b) $\mu/t = 2.4$. (c) $\mu/t = 1.8$. 
Figure 10: Static charge susceptibility $\chi_c(Q)$ and spin susceptibility $\chi_s(Q)$ for $U/t = 4$ and $T/t = 0.125$. The susceptibilities are plotted along the triangular Brillouin zone contour from $\Gamma \to X \to M \to \Gamma$, i.e., from $(0, 0) \to (\pi, 0) \to (\pi, \pi) \to (0, 0)$. Results are shown for the chemical potentials and site occupancies employed in Figure 5. Unless shown, statistical error bars are smaller than the plotting symbols. (a) $\chi_c(Q)$. (b) $\chi_s(Q)$. 

![Graph showing static charge susceptibility $\chi_c(Q)$ and spin susceptibility $\chi_s(Q)$ for $U/t = 4$ and $T/t = 0.125$.](image)
Figure 11: Static charge susceptibility $\chi_c(Q)$ and spin susceptibility $\chi_s(Q)$ for $U/t = 8$ and $T/t = 0.125$. The susceptibilities are plotted along the triangular contour used in Figure 10. Results are shown for the chemical potentials and site occupancies employed in Figure 6. (a) $\chi_c(Q)$. (b) $\chi_s(Q)$. 