Antiferromagnetic symmetry breaking in the half filled Hubbard model in infinite dimensions

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Abstract

We study the half filled Hubbard model on a hypercubic lattice in infinite dimensions in the presence of a staggered magnetic field. An exact Ward-identity between vertex functions and self-energies is derived, that holds in any phase without broken symmetry for all values of $U$. Making the reasonable assumptions that for small enough on-site repulsion $U$ the high-temperature phase is a Fermi liquid, and that in the weak coupling regime the effective Anderson impurity model can be studied perturbatively, we prove that Hartree-Fock theory and the random-phase approximation are very accurate for small $U$, and that the system develops long-range antiferromagnetic order at a finite temperature.

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I. INTRODUCTION

The physics of the Hubbard model in $d = \infty$ dimensions is currently investigated by several groups [1]-[9]. The essential simplification in infinite dimensions is that the self-energy $\Sigma(k, \omega)$ is independent of the wave vector $k$ [8]. At the same time, the dependence on the frequency $\omega$ remains non-trivial, and reflects generic features of correlated electronic systems. Recent works have mainly focused on Fermi liquid- and Mott insulating phases [1,2]. Although antiferromagnetic symmetry breaking has been briefly discussed in the literature [5,6], and has been studied numerically in Ref. [3], it seems that the functional-integral equations describing phases with broken symmetry have not been investigated analytically. A perturbative study of antiferromagnetism in infinite dimensions has recently been published in Ref. [9]. However, within this approach one finds at weak coupling a Neel temperature $T_N$ that is almost linear in the on-site repulsion $U$, in contradiction with Hartree-Fock theory, which predicts that $T_N$ is exponentially small. In the present work we shall use a non-perturbative method to study antiferromagnetic symmetry breaking in the repulsive half filled Hubbard model in infinite dimensions. We shall mainly focus on the weak coupling regime, and show that in this regime Hartree-Fock theory is essentially exact.

It is generally accepted that, at least in $d \geq 3$, the model has for any finite positive $U$ antiferromagnetic long-range order (LRO) at sufficiently low temperature. However, a rigorous proof of LRO does not exist. In particular, it is not obvious that the LRO is maintained for arbitrarily small $U > 0$, because the mean-field result for the order parameter at weak coupling is exponentially small, and fluctuations may be important. Here we shall consider Hubbard models with perfect nesting, particle-hole symmetry, and finite density of states at the Fermi energy. We shall proof that in $d = \infty$ there exists for sufficiently small but finite $U > 0$ a finite temperature $T_N(U) > 0$, such that the susceptibility for the staggered magnetization is divergent for all temperatures $T < T_N(U)$. Provided that no other susceptibility diverges at temperatures larger than $T_N$, our result implies the existence of long-range antiferromagnetic order in the weak coupling regime at low but finite temperatures.
One way to examine antiferromagnetic symmetry breaking is to calculate the staggered magnetization $M(h)$ in the presence of a staggered field $h$, take the thermodynamic limit, and then let $h \to 0$. If the spin-rotational symmetry is spontaneously broken, $M_0 \equiv \lim_{h \to 0} M(h)$ does not vanish. Alternatively, one can calculate the staggered susceptibility $\chi(T, U)$ in a parameter regime where $M_0 = 0$. Antiferromagnetic symmetry breaking manifests itself in a divergence of $\chi(T, U)$ at the Neel temperature $T_N(U)$. In the present work we shall take the latter approach and show that in infinite dimensions perfect nesting and particle-hole symmetry imply in the weak coupling regime that $T_N(U) > 0$ for $U > 0$.

The hamiltonian of the Hubbard models under consideration is given by $\mathcal{H} = \mathcal{H}_0 + \mathcal{U}$, with

$$
\mathcal{H}_0 = - \sum_{R,r} t_{r} c_{R+r}^\dagger c_{R} - h \cdot \sum_{R} c_{R}^\dagger \vec{\sigma} c_{R} e^{i \Pi \cdot R} \tag{1.1}
$$

$$
\mathcal{U} = U \sum_{R} \left[ c_{R+\uparrow}^\dagger c_{R+\uparrow} - \frac{1}{2} \right] \left[ c_{R+\downarrow}^\dagger c_{R+\downarrow} - \frac{1}{2} \right], \tag{1.2}
$$

where the $R$-sum is over $N$ sites of a $d$-dimensional hypercubic lattice, $h$ is a staggered field, and $\Pi = [\pi, \ldots, \pi]$ is the antiferromagnetic ordering vector (we set the lattice spacing equal to unity). We have defined two-component operators $c_{R}^\dagger = [c_{R+\uparrow}, c_{R+\downarrow}]$, where $c_{R+\sigma}^\dagger$ creates spin-$\sigma$ fermions at site $R$, and $\vec{\sigma} = [\sigma^x, \sigma^y, \sigma^z]$ are the Pauli matrices. We allow only hoppings that connect different sublattices, so that $e^{i \Pi \cdot r} = -1$. This implies that the band structure of the non-interacting model, defined by

$$
\epsilon_k = - \sum_{r} t_{r} e^{ik \cdot r} \tag{1.3}
$$

satisfies the perfect nesting condition

$$
\epsilon_{k+\Pi} = -\epsilon_k. \tag{1.4}
$$

Metzner and Vollhardt \cite{10} first pointed out that a non-trivial limit $d \to \infty$ is only obtained if the $t_{r}$ are properly rescaled with inverse powers of $d$ to compensate for the increase in the number of neighbors in high dimensions. The nearest neighbor hopping energy should be
scaled as $t_r = t/\sqrt{2d}$. For general hoppings connecting different sublattices, we require that

$t_r$ vanishes for large $d$ in such a way that for $d \to \infty$ the density of states at $U = 0$ has a finite limit $\rho(\epsilon)$,

\[
\rho(\epsilon) = \lim_{d \to \infty} \lim_{N \to \infty} \frac{1}{N} \sum_{\mathbf{k}} \delta(\epsilon - \epsilon_{\mathbf{k}}),
\]

where the wave-vector sum is over the first Brillouin zone. Note also that the hopping energies depend only in the distance between the sites, and do not break the translational invariance of the lattice. This is sufficient to assure that

\[
\rho(0) > 0.
\]

We have included the terms proportional to the density in the definition of the interaction in Eq.1.2, because then at half filling the chemical potential is exactly zero at any temperature, and the Hartree correction to the self-energy vanishes. The spectrum of our model has then particle-hole symmetry at half filling. The purpose of this paper is to show that this property, together with Eqs.1.4 and 1.6, are sufficient to imply that for $\rho(0)U \ll 1$ our model model has long-range antiferromagnetic order at sufficiently low but finite temperatures.

**II. ANTIFERROMAGNETISM IN INFINITE DIMENSIONS**

In this section we shall derive an exact functional-integral equation for the self-energies in the presence of a staggered field. Although an equivalent equation has been written down in Ref. [3], we use here an unconventional basis that greatly simplifies the following analysis.

Imposing the usual periodic boundary conditions, the free part $\mathcal{H}_0$ of our hamiltonian can be transformed into block-diagonal form via Fourier transformation,

\[
c_{\mathbf{k}\sigma} = N^{-1/2} \sum_{\mathbf{R}} e^{i\mathbf{k} \cdot \mathbf{R}} c_{\mathbf{R}\sigma}.
\]

Conventionally, one chooses the staggered field in the $z$-direction, $\mathbf{h} \cdot \vec{\sigma} = h\sigma^z$. In this case $\mathcal{H}_0$ can be written as
\[ H_0^z = \sum_{k \in RBZ} \sum_{\sigma} \tilde{C}_{k\sigma}^\dagger \begin{pmatrix} \epsilon_k & -\sigma h \\ -\sigma h & \epsilon_{k+\Pi} \end{pmatrix} \tilde{C}_{k\sigma}, \tag{2.2} \]

where the momentum sum is over the reduced Brillouin zone of the antiferromagnet, and \( \tilde{C}_{k\sigma}^\dagger = [c_{k\sigma}^\dagger, c_{k+\Pi\sigma}^\dagger]. \) Note that the sign of the off-diagonal elements in the quadratic form in Eq.2.2 depends on the spin projection. For a derivation of the functional integral-equation for the exact self-energy in \( d = \infty \) this introduces unpleasant technical difficulties, because we have to deal with two-component operators that carry in addition a spin index. A simple trick to avoid this difficulty is to choose the staggered field in the \( x \)-direction \([12], h \cdot \vec{\sigma} = h\sigma_x.\)

In this case Eq.1.1 can be written as

\[ H_0^x = \sum_k C_k^\dagger \begin{pmatrix} \epsilon_k & -h \\ -h & \epsilon_{k+\Pi} \end{pmatrix} C_k, \tag{2.3} \]

where the two-component operators are now defined by

\[ C_k^\dagger = [c_{k\uparrow}^\dagger, c_{k+\Pi\downarrow}^\dagger]. \tag{2.4} \]

Note that the \( C_k \) are composed from operators with different spin projection, and that the sum in Eq.2.3 is over the full Brillouin zone. Loosely speaking, the antiferromagnetic symmetry breaking is now labeled by a spin flip, so that the extra spin summation in Eq.2.2 can be absorbed in the second component of \( C_k. \) Of course, this is only a technical point, but it greatly facilitates the derivation of the functional-integral equation for the exact Greens function. In momentum space the interaction part of our hamiltonian can be written as

\[ U = \frac{U}{N} \sum_{k_1 \ldots k_4} \delta^*(k_1 + k_2 - k_3 - k_4) \]

\[ \times \left[ c_{k_1\uparrow}^\dagger c_{k_3\uparrow} - \frac{1}{2} \delta_{k_1,k_3} \right] \left[ c_{k_2+\Pi\downarrow}^\dagger c_{k_4+\Pi\downarrow} - \frac{1}{2} \delta_{k_2,k_4} \right], \tag{2.5} \]

where \( \delta_{k,k'} \) is the usual Kronecker-\( \delta, \) and \( \delta^*(k) = \sum_{\{K\}} \delta_{k,K}, \) where \( \{K\} \) are the vectors of the reciprocal lattice. In Eq.2.5 we have shifted the momentum of the last two operators by \( \Pi.\)
Obviously, this leaves $\delta^*$ invariant, so that the interaction term can be expressed entirely in terms of the components of the operator $C_k$ defined in Eq.\ref{eq:2.4}.

We now introduce the imaginary-time $2 \times 2$ matrix Greens function

$$G(k, \tau - \tau') = -<T C_k(\tau) C_k^\dagger(\tau')>,$$  \hspace{1cm} (2.6)

where $T$ denotes time ordering in imaginary time, and the time evolution and thermal average are determined by $\mathcal{H}_0^5 + \mathcal{U}$. The corresponding non-interacting Matsubara Greens function is

$$G^{(0)}(k, i\omega_n) = \int_0^{1/T} d\tau e^{i\omega_n\tau} G^{(0)}(k, \tau)$$

$$= \begin{pmatrix} i\omega_n - \epsilon_k & h \\ h & i\omega_n - \epsilon_{k+\Pi} \end{pmatrix}^{-1},$$  \hspace{1cm} (2.7)

where $\omega_n = \pi T (2n + 1)$. The self-energy matrix is defined as usual, $\Sigma(k, i\omega_n) = G^{(0)-1}(k, i\omega_n) - G^{-1}(k, i\omega_n)$. The essential simplification in $d = \infty$ is that the momentum conservation can be ignored \cite{8}, and we can replace $\delta^*(k) \to 1/N$ the mathematical expressions for the Feynman diagrams. The self-energy is then independent of $k$, and must be of the form

$$\lim_{d \to \infty} \Sigma(k, i\omega_n) \equiv \Sigma(i\omega_n) = \begin{pmatrix} \frac{\Sigma(i\omega_n)}{i\omega_n} & \frac{\Gamma(i\omega_n)}{\Sigma(i\omega_n)} \\ \frac{\Gamma(i\omega_n)}{\Sigma(i\omega_n)} & \frac{\Sigma(i\omega_n)}{i\omega_n} \end{pmatrix}.$$  \hspace{1cm} (2.8)

Particle-hole symmetry implies that

$$\Sigma(i\omega_n) = -\Sigma(-i\omega_n)$$  \hspace{1cm} (2.9)

$$\Gamma(i\omega_n) = \Gamma(-i\omega_n).$$  \hspace{1cm} (2.10)

The exact on-site Greens function is then given by

$$G_n = \frac{1}{N} \sum_k \left[ G^{(0)-1}(k, i\omega_n) - \Sigma_n \right]^{-1},$$  \hspace{1cm} (2.11)

where we use the abbreviation $G_n = G(i\omega_n)$ and $\Sigma_n = \Sigma(i\omega_n)$. From Eq.\ref{eq:2.7} it is clear that in general the summand on the left-hand side of Eq.\ref{eq:2.11} depends on $\epsilon_k$ and $\epsilon_{k+\Pi}$, and that
therefore the summation cannot be reduced to an integration over the density of states. However, if we require that the non-interacting band structure satisfies the perfect nesting condition, Eq. [1.4], the summand in Eq. [2.11] depends on $\epsilon_k$ only, so that

$$G_n = \int_{-\infty}^{\infty} d\epsilon n(\epsilon) \begin{pmatrix} i\omega_n - \epsilon - \Sigma_n & h - \Gamma_n \\ h - \Gamma_n & i\omega_n + \epsilon - \Sigma_n \end{pmatrix}^{-1}. \quad (2.12)$$

The unique signature of perfect nesting is that the energy $\epsilon$ enters in the upper- and lower diagonal elements with opposite sign.

The functional-integral equation for the exact Greens function is now derived in the standard way [8]. One defines a variational Greens function

$$\tilde{G}_n^{-1} = G_n^{-1} + \Sigma_n, \quad (2.13)$$

and a single-site impurity action

$$S_{imp} = -\frac{1}{T} \sum_n C_n^\dagger \tilde{G}_n^{-1} C_n + U \int_0^{1/T} d\tau \left[ n_\uparrow(\tau) - \frac{1}{2} \right] \left[ n_\downarrow(\tau) - \frac{1}{2} \right], \quad (2.14)$$

where $C_n^\dagger = [C_\uparrow^\dagger(\tau), C_\downarrow^\dagger(\tau)]$ are imaginary-time two-component Grassmann fields, with Matsubara components $C_n = T \int_0^{1/T} d\tau e^{i\omega_n \tau} C(\tau)$, and $n_\sigma(\tau) = C_\sigma^\dagger(\tau)C_\sigma(\tau)$. The functional-integral equation for the self-energies $\{\Sigma_n\}$ is then a $2 \times 2$ matrix equation

$$G_n = -\frac{1}{T} \frac{\int \mathcal{D}\{C, C^\dagger\} \exp[-S_{imp}] C_n C_n^\dagger}{\int \mathcal{D}\{C, C^\dagger\} \exp[-S_{imp}]} \equiv -\frac{1}{T} < C_n C_n^\dagger >_{S_{imp}}. \quad (2.15)$$

Because $S_{imp}$ depends on all $\{\Sigma_n\}$, the right-hand side of Eq. [2.15] is in general a non-linear functional of the self-energies, while the left-hand side is a non-linear function of $\Sigma_n$. Hence, Eq. [2.15] is a very complicated non-linear functional-integral equation. To calculate $\Sigma_n$, one should first calculate the exact Greens function of the impurity model in Eq. [2.14] for general choice of the $\{\Sigma_n\}$, and obtain an explicit expression for the right-hand side of Eq. [2.15]. After that, one should solve the resulting non-linear integral equation. Of course, such
a calculation can only be performed numerically. However, to examine the possibility of symmetry breaking, it is not necessary the explicitly solve these equations.

III. STAGGERED SUSCEPTIBILITY AND VERTEX FUNCTION

Suppose that $G_n$ is a solution of Eq.2.15. In the presence of a symmetry breaking field, the exact Greens function is of the form

$$G_n = \begin{pmatrix} G_n & F_n \\ F_n & G_n \end{pmatrix},$$

where the anomalous Greens function $F_n$ is related to the staggered magnetization $M(h, T)$ of the underlying Hubbard hamiltonian via

$$M(h, T) = T \sum_n F_n = \sum_n < C_n^\dagger \sigma^x C_n >_{\text{imp}}.$$  

Note that antiferromagnetic symmetry breaking in the original Hubbard model translates into ferromagnetic symmetry breaking in the impurity model. Of course, the concept of antiferromagnetism is meaningless in a world consisting of two degrees of freedom. Because the impurity model is essentially zero-dimensional, no spontaneous symmetry breaking can occur in this model. Thus, the spin-susceptibility $\tilde{\chi}$ of the impurity model, defined via

$$\tilde{\chi}(T) = T \int_0^{1/T} d\tau \int_0^{1/T} d\tau' \times < C^\dagger(\tau) \sigma^x C(\tau) C^\dagger(\tau') \sigma^x C(\tau') >_{\text{imp}} ,$$

remains finite for all values of $T$ and $U$ [13]. However, $\tilde{\chi}$ is not identical with the staggered susceptibility $\chi$ of the Hubbard model, defined by

$$\chi(T) = \lim_{h \to 0} \frac{\partial M(h, T)}{\partial h} .$$

This is evident from the fact that the self-energies are complicated functions of the external field, so that the derivative in Eq.3.4 does not simply produce the correlation function in
Eq. 3.3. Below we shall make the relation between $\chi$ and $\tilde{\chi}$ precise, and show that the self-consistency condition, Eq. 2.13, assures that $\chi$ can diverge at a finite temperature, while $\tilde{\chi}$ remains finite.

To derive an expression for the staggered susceptibility of the Hubbard model, let us first assume that the hopping energies $t_r$ in Eq. 1.1 are only non-vanishing for nearest neighbor sites. In the weak coupling regime, the generalization to arbitrary hoppings, subject to the restrictions mentioned earlier, is trivial and will be given shortly. Setting $t_r = t/\sqrt{2d}$ for $r$ connecting neighboring sites, the density of states in $d = \infty$ is

$$\rho(\epsilon) = \rho_0 \exp \left[-\pi \rho_0^2 \epsilon^2 \right], \quad (3.5)$$

with $\rho_0 \equiv \rho(0) = [t \sqrt{2\pi}]^{-1}$. The integration in Eq. 2.12 can then be done analytically, and we find that the diagonal- and off-diagonal elements of $G_n$ are given by

$$G_n = -\pi \rho_0 R_n \frac{i\omega_n - \Sigma_n}{\Omega_n}, \quad (3.6)$$

$$F_n = \pi \rho_0 R_n \frac{h - \Gamma_n}{\Omega_n}, \quad (3.7)$$

where

$$\Omega_n = \left[-(i\omega_n - \Sigma_n)^2 + (h - \Gamma_n)^2 \right]^{1/2}, \quad (3.8)$$

$$R_n = \text{erfc} \left[ \sqrt{\pi \rho_0 \Omega_n} \right] \exp \left[ \pi \rho_0^2 \Omega_n^2 \right]. \quad (3.9)$$

Here erfc$[x]$ is the complimentary error function, and the root in Eq. 3.8 should be taken such that $\text{Re} \Omega_n \geq 0$. The leading terms of $R_n$ for small and large $\rho_0 |\Omega_n|$ is

$$R_n \sim \begin{cases} 1 & \text{for } \rho_0 |\Omega_n| \ll 1 \\ [\pi \rho_0 \Omega_n]^{-1} & \text{for } \rho_0 |\Omega_n| \gg 1 \end{cases}. \quad (3.10)$$

Thus, $R_n$ acts as a high-energy cutoff for frequency summations. As long as the Matsubara sums are dominated by the infrared regime $\rho_0 |\omega_n| \ll 1$, the precise form of the cutoff is irrelevant, so that we may set $R_n = 1$, keeping in mind that all frequency sums are cut off by an energy of the order of $\rho_0^{-1}$. 

9
It is now also clear that inclusion of hoppings between the sublattices beyond the nearest neighbors will lead to a different value of the cutoff \( \rho_0 \), and a different functional form of the function \( R_n \) at high frequencies. However, the low-frequency behavior of Eqs.3.6-3.8 will be unchanged, because the form of these equations carries the unique signature of perfect nesting, and is in this sense universal. Hence, for \( \rho_0 U \ll 1 \) all calculations presented below hold also for arbitrary hoppings, provided we substitute the value of \( \rho_0 \) and the cutoff function \( R_n \) corresponding to the particular choice of hoppings.

To examine the stability of the paramagnetic phase, we now calculate the staggered susceptibility \( \chi \). Substituting Eq.3.7 into Eq.3.2, differentiating with respect to \( h \) and letting \( h \to 0 \), we obtain an exact relation between the staggered susceptibility and the self-energy of the Hubbard model

\[
\chi = T \sum_n \chi_n \tag{3.11}
\]

\[
\chi_n = \lim_{h \to 0} \frac{\partial F_n}{\partial h} = \pi \rho_0 R_n \frac{\Lambda_n}{\Omega_n} , \tag{3.12}
\]

where we have used the fact that in a parameter regime in which the symmetry is not spontaneously broken \( \lim_{h \to 0} \Gamma_n = 0 \). It is understood that \( \Omega_n \) and \( R_n \) are now defined by setting \( h = \Gamma_n = 0 \) in Eqs.3.8 and 3.9. The vertex function \( \Lambda_n \) is defined via the Ward-identity

\[
\Lambda_n = 1 - \lim_{h \to 0} \frac{\partial \Gamma_n}{\partial h} . \tag{3.13}
\]

The divergence of the susceptibility is controlled by the low-frequency behavior of the self-energies. Recently it has been convincingly demonstrated that in the weak coupling regime the phase without broken symmetry is a Fermi liquid [1,2,4]. Assuming that this is indeed correct, we now show that for \( \rho_0 U \ll 1 \) the staggered susceptibility diverges in the limit \( T \to 0 \).

Particle-hole symmetry implies \( \Sigma(0) = 0 \), see Eq.2.9. The infrared behavior of the sum in Eq.3.11 is then determined by the finite temperature effective mass- and vertex renormalization factors \( Z_\omega = m/m^* \) and \( Z_h \),

10
\[ Z_\omega^{-1} = 1 - \frac{\text{Im}\Sigma_0}{\omega_0} \]  \hspace{1cm} (3.14)
\[ Z_h^{-1} = 1 - \lim_{h \to 0} \frac{\partial \Gamma_0}{\partial h} . \]  \hspace{1cm} (3.15)

Note that \( Z_h^{-1} \) is precisely the zero-frequency limit of the vertex defined in Eq.3.13. From 2.10 it is clear that \( \Lambda(i\omega_n) \) is an even function of frequency, so that the low-frequency behavior of Eq.3.11 is determined by \( \Lambda_0 \). We emphasize that in the strong-coupling regime \( \rho_0 U \gtrsim 1 \) the phase without broken symmetry is most likely a Mott insulator, where Fermi liquid theory is not valid, and the effective mass diverges \([1,2,4]\). Therefore our proof is necessarily restricted to the weak coupling regime. Combining Eq.3.14 with Eq.3.8, we obtain for small frequencies

\[ \Omega_n \sim Z_\omega^{-1}|\omega_n| . \]  \hspace{1cm} (3.16)

Substituting Eq.3.16 into Eq.3.12, we see that in the weak coupling regime the susceptibility is to leading logarithmic order given by

\[ \chi = \rho_0 \frac{Z_\omega}{Z_h} [L + O(1)] , \]  \hspace{1cm} (3.17)

where the dimensionless factor \( L \) is in the low temperature regime \( \rho_0 T \ll 1 \) given by

\[ L = \pi T \sum_n R_n \frac{1}{|\omega_n|} = \ln (\rho_0 T)^{-1} + O(1) . \]  \hspace{1cm} (3.18)

Note that \( R_n \) merely provides a high-energy cutoff of the order of \( \rho_0^{-1} \) to the Matsubara sum, the precise value of which is irrelevant. Eq.3.17 is completely general, although all interesting physics is hidden in the renormalization factors \( Z_\omega \) and \( Z_h \). Without further explicit knowledge of these factors, there are a priori two possibilities: The first is that \( Z_\omega/Z_h \) diverges at a finite \( T > 0 \). Below we shall show that in the regime \( 0 < \rho_0 U \ll 1 \) this is indeed the case, because \( Z_h \) vanishes while \( Z_\omega \) remains finite. The second possibility is that \( Z_\omega/Z_h \) remains finite. It turns out that, at least in the weak coupling regime, this is only true for \( U = 0 \), where \( Z_\omega = Z_h = 1 \). In this case the divergence of the susceptibility is due to the divergence of \( L \) as \( T \to 0 \). In both cases, however, \( \chi = \infty \) at \( T = 0 \). Note the essential
role of particle-hole symmetry to assure that $\Omega_n$ vanishes in the limit $\omega_n \to 0$, so that the infrared cutoff for the sum in Eq. 3.18 is $\omega_0 = \pi T$, and no other energy scale. The only way in which the divergence could be avoided is via a divergence of the effective mass, so that $Z_\omega = 0$. This possibility can be excluded, because the weak coupling phase without broken symmetry is by assumption a Fermi liquid. We therefore conclude that the antiferromagnetic susceptibility is always infinite at $T = 0$. This is of course due to the nesting instability built into our model. Hence, the zero-temperature divergence of the staggered susceptibility survives in the weakly interacting theory, and leads to an antiferromagnetic ground state with spontaneously broken symmetry. This is the first main result of this work. Of course, we cannot exclude the possibility that some other susceptibility exhibits an even stronger divergence, but this seems to be very unlikely.

IV. WARD-IDENTITY AND PROOF OF SYMMETRY BREAKING FOR $T > 0$

AT WEAK COUPLING

To proof that $T_N(U) > 0$, we now show that $Z_h$ vanishes for $U > 0$ at a finite temperature. To get some intuition how this might happen, let us first calculate $Z_h$ within Hartree-Fock theory. In this approximation the self-energies are independent of frequency, so that $\Sigma_n = 0$ by particle-hole symmetry, and $Z_\omega = 1$. The off-diagonal self-energy is given by the first-order exchange diagram,

$$\Gamma^{(1)} = -UT \sum_n F_n^{(1)}$$

where $F_n^{(1)}$ is obtained from our general expression in Eq. 3.7 by setting $\Sigma_n = 0$ and $\Gamma_n = \Gamma^{(1)}$. Note that Eq. 4.1 is the usual self-consistency equation for the mean-field gap $\Delta \equiv -\Gamma^{(1)}$. At low temperatures Eq. 4.1 reduces to

$$\Gamma^{(1)} = \rho_0 U L [\Gamma^{(1)} - h]$$

where the $L$ is defined in Eq. 3.18. Differentiating both sides of Eq. 4.2 with respect to $h$ and letting $h \to 0$ yields
\[ Z_h = 1 - \rho_0 U L \quad . \] (4.3)

The mean-field estimate for the Neel temperature is then obtained from \( Z_h = 0 \), which yields

\[ T_N \propto \rho_0^{-1} \exp \left[ - (\rho_0 U)^{-1} \right] \quad . \] (4.4)

From Eqs.3.11, 3.12 and 4.3 it is also obvious that the Hartree-Fock approximation for the self-energies leads to the random-phase approximation for the susceptibility.

To show that Hartree-Fock theory is qualitatively correct, we now derive an integral equation for the vertex function \( \Lambda_n \). The crucial observation is that \( Z_h \) can be determined by differentiation of the self-consistency equation for the self-energies. The Hartree-Fock self-consistency requirement, Eq.4.1, is the simplest possible approximation. In infinite dimensions we have an exact self-consistency equation at our disposal. The obvious procedure is then to differentiate the off-diagonal components of both sides of the functional-integral equation, Eq.2.15, with respect to \( h \), and taking then the limit \( h \to 0 \). After a simple calculation we obtain in this way an exact integral equation for the vertex function \( \Lambda_n \)

\[
2\pi\rho_0 R_n \frac{\Lambda_n}{\Omega_n} = \sum_m \tilde{\chi}_{n,m} \left[ 1 + \Lambda_m \left( \frac{1}{\pi\rho_0 R_m \Omega_m} - 1 \right) \right],
\] (4.5)

where the kernel \( \tilde{\chi}_{n,m} \) is the following correlation function of the impurity model,

\[
\tilde{\chi}_{n,m} = \frac{1}{T^2} \langle C_n^{\dagger} \sigma^x C_n C_m^{\dagger} \sigma^x C_m \rangle_{\text{imp}}.
\] (4.6)

Eq.4.3 is valid for all values of \( U \) and temperatures \( T > T_N(U) \). The kernel of this integral equation is given by the Matsubara components \( \tilde{\chi}_{n,m} \) of the susceptibility of the impurity model. The \( \tilde{\chi}_{n,m} \) do not have a direct physical meaning, and should be considered as auxiliary quantities. The susceptibility of the impurity model, defined in Eq.3.3, can be written in a form analogous to Eqs.3.11 and 3.12.

\[
\tilde{\chi} = T \sum_n \tilde{\chi}_n \quad .
\] (4.7)

\[
\tilde{\chi}_n = \sum_m \tilde{\chi}_{n,m} = \frac{1}{T^2} \sum_m \langle C_n^{\dagger} \sigma^x C_n C_m^{\dagger} \sigma^x C_m \rangle_{\text{imp}}.
\] (4.8)
Of course, we do not have an analytic expression for $\tilde{\chi}_{n,m}$, but for $\rho_0 U \ll 1$ this kernel can in principle be calculated perturbatively, and is free of singularities [14].

To determine $Z_h$, we multiply both sides of Eq.4.5 by $T$ and sum over $n$. By construction, summation of the left-hand side of Eq.4.5 yields precisely $2\chi$, see Eqs.3.11 and 3.12. Recalling that $Z_h^{-1}$ is by definition the zero-frequency limit of the vertex $\Lambda_n$, we obtain from Eq.4.5

$$2\chi = \tilde{\chi} + Z_h^{-1} T \sum_n \tilde{\chi}_n \lambda_n \left[ \frac{1}{\pi \rho_0 R_n \Omega_n} - 1 \right] , \quad (4.9)$$

where

$$\lambda_n = \frac{\Lambda_n}{\Lambda_0} = 1 - \frac{\Lambda_0 - \Lambda_n}{\Lambda_0} . \quad (4.10)$$

Re-arranging terms, (4.9) can be written as

$$Z_h = Z - \tilde{\chi}^{-1} \left[ T \sum_n \frac{\lambda_n}{\pi \rho_0 R_n \Omega_n} \tilde{\chi}_n - 2Z_h\chi \right] , \quad (4.11)$$

with the numerical constant $Z$ given by

$$Z = \frac{\sum_n \lambda_n \tilde{\chi}_n}{\sum_n \tilde{\chi}_n} . \quad (4.12)$$

In the non-interacting limit a simple calculation of the vertex function $\tilde{\chi}_n$ defined in Eq.4.8 gives

$$\tilde{\chi}_n^{(0)} = -2G_n^{(0)2} = 2\pi^2 \rho_0^2 R_n^{(0)2} , \quad (4.13)$$

where $R_n^{(0)}$ is the value of $R_n$ at $U = 0$, and

$$G_n^{(0)} = -i\pi \rho_0 R_n^{(0)} \text{sign} \omega_n \quad (4.14)$$

is the non-interacting Greens function, see Eq.3.6. Combining Eq.4.13 with Eqs.3.11 and 3.12, we obtain the exact identity

$$2Z_h\chi = T \sum_n \lambda_n R_n \tilde{\chi}_n^{(0)} \frac{1}{\pi \rho_0 \Omega_n R_n^{(0)2}} . \quad (4.15)$$

Substituting Eq.4.15 into Eq.4.11, we finally we arrive at
\[ Z_h = Z - \frac{T}{\chi} \sum_n \frac{\lambda_n R_n}{\pi \rho_0 \Omega_n} \sum \left[ \frac{\tilde{\chi}_n}{R_n^2} - \left( \frac{\tilde{\chi}_n}{R_n^2} \right)_{U=0} \right]. \]  

(4.16)

This equation is the central result of this work. It has the structure of a Ward-identity, relating a vertex function (i.e. a derivative of a Greens function) to the Greens function itself. This identity is a direct consequency of the fact that in infinite dimensions the exact local Greens function satisfies a self-consistency condition. Note that \( Z_h = 1/\Lambda_0 \) appears also on the right hand side of Eq.4.16. However, \( \Lambda_0 \) appears exclusively through the regularized combination \( \lambda_n = 1 - (\Lambda_0 - \Lambda_n)/\Lambda_0 \), which deviates from unity only due to the non-trivial frequency dependence of the self-energies, and remains manifestly finite even if \( \Lambda_0 \) diverges.

From Eqs.4.10 and 2.10 it is obvious that for small \( U \) and \( \omega_n \) we have \( \lambda_n = 1 + O(U^2 \omega_n^2) \). Therefore all quantities on the right-hand side of Eq.4.16 are free of singularities, and can be calculated perturbatively if \( \rho_0 U \ll 1 \). To obtain the leading logarithmic divergence of the sum in Eq.4.16, we can safely ignore vertex corrections and set \( \lambda_n = 1 \).

From Eq.4.16 it is clear that \( U = 0 \) is a singular point in parameter space, because only in this case the enumerator in the last term vanishes, so that \( Z_h = Z = 1 \). For any finite \( U \), the singular frequency dependence in the last term in Eq.4.16 leads in the zero-temperature limit to an infrared divergence.

We emphasize that Eq.4.16 is exact and valid for all values of \( U \) and \( T \), as long as the symmetry is not spontaneously broken. Note also the formal similarity with the Hartree-Fock result. In fact, if the right-hand side of Eq.4.16 is expanded to first order in \( \rho_0 U \), we recover Eq.4.3. In this approximation \( \Lambda_n \) is independent of \( n \), so that \( \lambda_n = 1 \). From Eq.4.12 we see that this implies also \( Z = 1 \). Straight-forward perturbation theory gives to first order in \( U \)

\[ \tilde{\chi}_n = \chi_n^{(0)} - UG_n^{(0)2}T \sum \chi_m^{(0)} + O(U^2) \]  

(4.17)

Using then Eq.4.14, we see that

\[ \tilde{\chi}^{-1} \left[ \frac{\tilde{\chi}_n}{R_n^2} - \left( \frac{\tilde{\chi}_n}{R_n^2} \right)_{U=0} \right] = \pi^2 \rho_0^2 U + O(U^2), \]  

(4.18)
and finally

\[ Z_h = 1 - \rho_0 U \pi T \sum_n \frac{R_n}{|\omega_n|} \times [1 + O(\rho_0 U)] . \]  

(4.19)

This is precisely the Hartree-Fock result, which has been derived above in a much simpler way, see Eq.4.13. However, Eq.4.16 is completely rigorous, and contains all quantum fluctuations neglected in Hartree-Fock theory.

We now use the well known properties of the impurity model to show that the Hartree-Fock value for the Neel temperature is asymptotically exact in the limit \( \rho_0 U \to 0 \). The right-hand side of Eq.4.16 depends on the self-energies \( \Sigma_n \), the vertices \( \lambda_n \), and the susceptibilities \( \tilde{\chi}_n \) of the impurity model, which by virtue of Eq.2.15 can also be considered as functionals of the self-energies. The crucial point is now that all these quantities can in principle be calculated perturbatively in powers of \( \rho_0 U \), and that the perturbation theory has a finite radius of convergence. This follows from the facts (i) that our model is by assumption a Fermi liquid, so that all interaction effects can be absorbed in finite renormalization factors. The second cornerstone of our proof is the fact (ii) that the Anderson impurity model can be treated perturbatively in the weak coupling regime. The lowest order correction to the impurity susceptibility is given by Eq.4.18. For impurity models with non-interacting Greens function of the form \( \tilde{G}^{(0)}_n = [i\omega_n + i\Delta \text{sign}\omega_n]^{-1} \) Zlatić and Horvatić [14] have proven that the perturbation series for the spin susceptibility is absolutely convergent for any \( |U| < \infty \), and that in the weak coupling regime the first few terms of the series yield an extremely accurate approximation of the exact result. Although the self-consistent Greens function \( \tilde{G}_n \) in Eq.2.14 will not be of the form assumed in Ref. [14], it is extremely plausible that the validity of perturbation theory does not depend on the precise form of the non-interacting Greens function [1].

Eqs.4.15 and 4.12 imply that for small enough \( U \) the constant \( Z \) has a convergent expansion with the first two terms given by

\[ Z = 1 + z_1 (\rho_0 U)^2 + \ldots , \]  

(4.20)
where the constant \( z_1 \) is of the order of unity. Moreover, particle-hole symmetry guarantees that the infrared cutoff for the sum in Eq. 4.16 is \( \Omega_0 = \pi T/Z_\omega \), so that the sum is logarithmically divergent in the limit \( T \to 0 \). Hence, the last term in Eq. 4.16 can be made arbitrarily large by choosing the temperature small enough, provided that \( U > 0 \) and the effective mass renormalization \( Z_\omega \) remains finite. Consequently, for arbitrarily small but positive \( U \) there exists always a temperature \( T_N > 0 \) such that \( Z_h \) vanishes.

It follows by continuity that the Hartree-Fock result becomes asymptotically exact for \( \rho_0 U \to 0 \), and that therefore Hartree-Fock theory correctly predicts a finite staggered magnetization in the weak coupling regime. The Neel temperature \( T_N(U) \) can in principle be calculated by expanding \( \Sigma_n, \lambda_n, \) and \( \tilde{\chi}_n \) to the desired order in \( \rho_0 U \), and finding the temperature that satisfies

\[
\sum_n \lambda_n \tilde{\chi}_n = \sum_n \frac{\lambda_n R_n}{\pi \rho_0 \Omega_n} \left[ \tilde{\chi}_n \frac{R_n}{R_n^2} - \left( \frac{\tilde{\chi}_n R_n^2}{R_n^2} \right)_{U=0} \right].
\]

Because for small \( \rho_0 U \) the solution of this equation smoothly connects with the Hartree-Fock result, it has, at least for small enough \( \rho_0 U \), a finite solution \( T_N > 0 \). This completes our proof that the Hubbard model in infinite dimensions has indeed a finite Neel temperature in the weak coupling regime. Combining Eqs. 3.17 and 4.16, we obtain the following exact result for the staggered susceptibility in the regime \( T, U \ll \rho_0^{-1} \),

\[
\chi = \frac{\rho_0 Z_\omega \ln (\rho_0 T)^{-1}}{Z - \frac{T}{\chi} \sum_n \frac{\lambda_n R_n}{\pi \rho_0 \Omega_n} \left[ \tilde{\chi}_n \frac{R_n}{R_n^2} - \left( \frac{\tilde{\chi}_n R_n^2}{R_n^2} \right)_{U=0} \right]}. \tag{4.22}
\]

Note that the form of this equation is very similar to the standard result of the random-phase approximation. In fact, to leading order in \( \rho_0 U \) Eq. 4.22 reduces precisely to the random-phase approximation. In fact, to leading order in \( \rho_0 U \) Eq. 4.22 reduces precisely to the random-phase approximation for \( \chi \).

**V. CONCLUSIONS**

The existence of an antiferromagnetic instability in the weak coupling regime of the half filled Hubbard models with perfect nesting is not surprising. Such an instability is predicted
by Hartree-Fock theory in all dimensions. While in one dimension this instability is known
to be an artifact of mean-field theory, conventional wisdom is that at least in high enough
dimensions Hartree-Fock theory becomes very accurate. In the present work we have used
the machinery available in infinite dimensions to show that for $\rho_0 U \ll 1$ Hartree-Fock theory
and the random-phase approximation are very accurate in $d = \infty$. We have shown that the
particle-hole symmetry of the half filled model, together with the perfect nesting property
of the non-interacting energy dispersion, determine the behavior of the susceptibility at low
temperatures. By differentiation of the exact self-consistency condition available in $d = \infty$,
we have obtained exact Ward-identities between vertex functions and self-energies. The
central equations, Eqs.4.5 and 4.16, hold for all values of $T$ and $U$ as long as the symmetry is
not spontaneously broken, and are the basis for our proof of the antiferromagnetic instability
in the weak coupling regime. To show that the Neel temperature is indeed finite, we have
assumed (i) that the high-temperature phase without broken symmetry is a Fermi liquid.
For small enough $\rho_0 U$ this assumption can be justified by recent analytical and numerical
work [1,2,4]. Another essential ingredient in our proof is (ii) that in the weak coupling
limit the susceptibility of the impurity model can be calculated perturbatively and reduces
to the susceptibility of the non-interacting theory in a continuous and smooth way. Both
assumptions, (i) and (ii), are on solid grounds [14] and can hardly be questioned. If the
reader is willing to accept these assumptions, then our proof can be considered as rigorous.

We have not made any prediction about the strong coupling phase. Although our funda-
mental equations are also valid in this case, the analysis becomes more difficult, because
self-energies and impurity susceptibilities cannot be calculated by straight-forward expansion
in powers of $U$. In particular, for $\rho_0 U \gtrsim 1$ we expect that the phase without broken
symmetry is a Mott insulator, with diverging effective mass [1,2]. Thus, if the ground
state at strong coupling is an antiferromagnet (at least for nearest neighbor hopping this
is certainly the case), then we expect a direct transition between a Mott insulator and an
antiferromagnet as we lower the temperature. The analysis of Eqs.4.5, 4.16, and Eq.4.21,
which are of course also valid at strong coupling, might reveal interesting new phenomenas,
and is left for the future.

What is the relevance of our result to finite dimensions? For \( d < \infty \) the density of states \( \rho(\epsilon) \) vanishes outside a fixed interval. However, we have seen that in the weak coupling regime the only parameter that determines the infrared behavior of Matsubara sums is \( \rho(0) \). Therefore, we believe that in all dimensions \( d \geq 3 \) the Hartree-Fock theory becomes asymptotically exact for \( \rho_0 U \to 0 \). Obviously our result does not extrapolate to \( d = 1 \). But in this case the Hubbard model can be solved exactly, and we know that there is no spontaneous magnetization for all \( U \), even at \( T = 0 \) \[15\]. In \( d = 2 \) Hartree-Fock theory is completely incorrect at \( T > 0 \), because it predicts spontaneous symmetry breaking at low temperatures, although the rigorous Mermin-Wagner theorem \[16\] tells us that this can happen only at \( T = 0 \). Note also that in two dimensions \( \rho(0) = \infty \) due to Van Hove singularities. Thus, at weak coupling the extrapolation of the physics in \( d = \infty \) to \( d = 2 \) is not possible. For nearest neighbor-hopping and large \( U \), the half filled square lattice Hubbard model is equivalent to a two dimensional quantum Heisenberg antiferromagnet, which seems to be ordered at \( T = 0 \). There remains the possibility that the order in the ground state is destroyed in the weak coupling regime \[17,18\]. It can be shown \[19\] that even for arbitrarily small \( U \) the perturbation expansion is not governed by a small parameter, and that, in contrast to \( d \geq 3 \), all ”perturbative” corrections to Hartree-Fock theory in \( d = 2 \) are of the relative order of unity. Thus, \( d = 2 \) seems to be closer to \( d = 1 \), and a simple Hartree-Fock description of the weak coupling regime seems not to be justified.

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