HELCITY MODULUS
AND
EFFECTIVE HOPPING
IN THE
TWO-DIMENSIONAL HUBBARD MODEL
USING SLAVE-BOSON METHODS.

P.J.H. Denteneer and M. Blaauboer
Instituut-Lorentz, University of Leiden,
P. O. Box 9506, 2300 RA Leiden, The Netherlands

Abstract

The slave-boson mean-field method is used to study the two-dimensional Hubbard model. A magnetic phase diagram allowing for paramagnetism, weak- and strong ferromagnetism and antiferromagnetism is constructed and compared to the corresponding phase diagram using the Hartree-Fock approximation (HFA). Magnetically ordered regions are reduced by a factor of about 3 along both the $t/U$ and density axes compared to the HFA. Using the spin-rotation invariant formulation of the slave-boson method the helicity modulus is computed and for half-filling is found to practically coincide with that found using variational Monte Carlo calculations using the Gutzwiller wave function. Off half-filling the results can be used to compare with Quantum Monte Carlo calculations of the effective hopping parameter. Contrary to the case of half-filling, the slave-boson approach is seen to greatly improve the results of the HFA when off half-filling.

PACS: 75.10.Lp, 71.27.+a, 64.60.-i

Short title: Helicity modulus in the Hubbard model using slave bosons
1 Introduction

In the study of correlated electrons, for which both charge and spin degrees of freedom are relevant, the Hubbard model is an intriguing simplification of reality that still contains a great deal of the essential physics [1]. Although superconductivity has not been demonstrated in this model, it is able to explain or reproduce a large number of experimental results on the copper oxides which superconduct at high temperatures [2]. Despite such encouraging results, understanding of the model in dimensions two and higher is still rather limited. Even when the most elementary mean-field approximation, the Hartree-Fock approximation, is invoked, the phase diagram cannot be determined in full [3], since inhomogeneous phases, like spiral phases or domain walls, are able to supersede simple ferro- or antiferromagnetic phases. The possibility exists that more complicated phases not considered so far are also important. Rigorous techniques like Quantum Monte Carlo and exact diagonalization are limited to temperatures which may be too high and lattices which may be too small, respectively. Therefore it is of interest to employ approximations which go beyond the Hartree-Fock approximation (HFA).

Some years ago Kotliar and Ruckenstein introduced, for the Hubbard model, the technique of using slave bosons to keep closer track of the site-occupancy than is done in the HFA. If a further approximation is made, the so-called “slave-boson mean-field” (SBMF) approximation, this approach was shown to be equivalent to the approximation scheme of Gutzwiller for the Hubbard model [4]. In a parallel development it was shown by Vollhardt and co-workers that the Gutzwiller approximation scheme becomes exact in the limit of an infinite number of spatial dimensions, whereas the HFA does not become exact in this limit [5, 6]. Therefore, just like in classical statistical physics mean-field theory is a good starting point to study a specific model (because fluctuations become increasingly less relevant when increasing the dimension), for quantum models the SBMF approximation is a good starting point. In any case, it is expected to be an improvement over the HFA. In this connection, it is of interest to note that Oleś and Zaanen compared the Gutzwiller approximation (GA) with the HFA in a two-band model of copper-oxide planes and showed that the GA is a good approximation for correlations at small length scales [7]. More recently the slave-boson approach of Kotliar and Ruckenstein has been refined in order to make it spin-rotation invariant [8, 9].

In this paper, we make a detailed comparison of the SBMF and Hartree-Fock approximations to the (one-band) Hubbard model on a two-dimensional square lattice. Where possible we also compare to Quantum Monte Carlo calculations. By using the analytical result for the density of states of freely hopping electrons on the square lattice all calculations can conveniently be performed for a lattice of infinite size using one-dimensional integrals (over energy) only. Although we will mostly present results for the ground state ($T = 0$), the formulation we present is to a large extent valid for finite temperatures as well. A further advantage of the SBMF approach is that, in principle, it is valid for the whole range of Hubbard repulsion strengths and electron densities. First, we construct a ground-state phase-diagram allowing only for the simple magnetic phases: paramagnetic, antiferromagnetic, weakly and strongly (i.e. partially and fully polarized) ferromagnetic. We determine
all first-order and continuous transitions between these phases. Although this approach may not give much information on the exact phase diagram (for instance, it is known that phases with spiraling magnetization supersede the antiferromagnet when going off half-filling), it gives a clear impression of the improvement of the SBMF approximation over the HFA. Next, we derive an expression for the helicity modulus or spin stiffness in SBMF approximation using the spin-rotation invariant formulation and compare (for half-filling) to previous calculations of the helicity modulus in the HFA, as well as using the Gutzwiller wave function in a variational Monte Carlo calculation \[^1\]. It turns out that in SBMF approximation, apart from a negligible contribution, the helicity modulus is completely determined by the average kinetic energy (as is the case in the HFA) and therefore equivalent to the effective hopping parameter. When comparing the SBMF results for the effective hopping parameter to HFA and QMC calculations the improvement with respect to the HFA is only a few percent at half-filling and practically coincides with the results of variational Monte Carlo calculations using the Gutzwiller wave function, but the improvement is substantial off half-filling.

The paper is organised as follows: in Section 2, we briefly introduce the slave-boson mean-field method for the Hubbard model and present the free energy for the antiferromagnetic, ferromagnetic and spiral phases as well as the corresponding consistency equations. In Section 3, we construct the ground-state phase diagram for the simple magnetic phases listed above and compare to the corresponding HFA phase diagram. An expression for the helicity modulus is derived and its connection to the effective hopping parameter is discussed in Section 4. The SBMF results are compared to both the HFA and QMC calculations where possible. The last section contains a discussion of the results and draws some conclusions.

2 Slave Boson Mean Field method

The Hamiltonian for the Hubbard model is given by:

\[ H = - \sum_{ij\sigma} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + U \sum_i n_{i\uparrow}n_{i\downarrow} - \mu \sum_i n_{i\sigma}, \]  

(1)

where \( c_{i\sigma}^\dagger \) creates an electron at site \( i \) with spin \( \sigma \), \( n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma} \), \( t_{ij} \) is the one-electron transfer integral between sites \( j \) and \( i \) (\( t_{ij} \) equals \( t \) if \( i \) and \( j \) are nearest neighbours and 0 otherwise), \( U \) the on-site repulsion (\( U > 0 \)), and \( \mu \) the chemical potential (\( \mu = U/2 \) corresponds to a half-filled lattice, i.e. \( n = \sum_\sigma \langle n_{i\sigma} \rangle = 1 \)).

The Hubbard model allows for four different occupancies of a single site: it can be empty, singly occupied by either a spin-up or spin-down electron, or doubly occupied (by electrons of opposite spin). This leads to the idea of introducing four different kinds of “slave” bosons, one for each of the possible occupancies. In order for this to become a bookkeeping device one introduces the constraints that at each site there is always exactly one boson present and that it is of the kind corresponding to the electron occupancy. If \( e, p_\uparrow, p_\downarrow \) and \( d \) denote the annihilation
operators for the four kinds of bosons, these constraints are:

\[ e_i^\dagger e_i + \sum_{\sigma} p_{i\sigma}^\dagger p_{i\sigma} + d_i^\dagger d_i = 1 \quad \text{for all } i, \]  
\[ c_{i\sigma}^\dagger c_{i\sigma} = p_{i\sigma}^\dagger p_{i\sigma} + d_i^\dagger d_i \quad \text{for all } i \text{ and } \sigma = \uparrow, \downarrow, \]  

(2)

(3)

The interaction term in the Hamiltonian (1) can now be replaced by one containing only the counting operator for \( d \)-bosons. In order for the boson presence to keep in correspondence with the electron occupancy for each site, the hopping term in the Hamiltonian needs to be adjusted by connecting to each electron annihilation operator \( c_{i\sigma} \) the following boson-transformation operator:

\[ \tilde{z}_{i\sigma} = e_i^\dagger p_{i\sigma} + p_{i,-\sigma}^\dagger d_i. \]

(4)

In fact this choice for \( \tilde{z} \) is not unique [14] and we follow Ref. [4] by making a choice which in the case of \( U = 0 \) gives the correct result if a subsequent saddle-point approximation is made:

\[ z_{i\sigma} = \left(1 - d_i^\dagger d_i - p_{i\sigma}^\dagger p_{i\sigma}\right)^{-\frac{1}{2}} \tilde{z}_{i\sigma} \left(1 - e_i^\dagger e_i - p_{i,-\sigma}^\dagger p_{i,-\sigma}\right)^{-\frac{1}{2}}. \]

(5)

In the physical subspace, defined by (2)-(3), of the enlarged boson-electron Hilbert space, the Hamiltonian,

\[ \mathcal{H}_{SB} = -\sum_{ij\sigma} t_{ij} \zeta_{i\sigma}^\dagger \zeta_{j\sigma} + U \sum_i d_i^\dagger d_i - \mu \sum_i n_{i\sigma}, \]

(6)

has the same matrix elements as the original Hamiltonian in the original Hilbert space containing only electron states. Therefore, up to here only a reformulation of the original problem has been achieved. However, if now in the functional integral formulation the saddle-point approximation of time- and position-independent Bose fields is made, a set of equations results which is similar to those found in the Hartree-Fock approximation, but more general. This approximation is called the Slave-Boson Mean-Field (SBMF) approximation. For comparison, the HFA can be obtained in such a functional integral formulation by first applying a suitable Hubbard-Stratonovich transformation and then making the saddle-point approximation for the original problem [13]. For further details on the functional integral formulation for the Hubbard model and the subsequent saddle-point approximation we refer to previous papers on this subject [4, 8, 9, 14, 16].

In the next three subsections, we present the expressions for the free energy of the ferromagnetic, antiferromagnetic, and spiral phases. For the ferromagnet and antiferromagnet we also give the consistency equations for the appearing self-consistent fields, which must be obeyed for the free energy to become minimal. To some extent this is a repetition of previously published results [10, 16], but they are given for the reader’s convenience and to establish the notation.

### 2.1 Ferromagnetic Phase

For the ferromagnetic phase one assumes a non-zero homogeneous magnetization \( m \), even if a magnetic field is absent. To be able to calculate the magnetic susceptibility
we also include a magnetic field $h$ in the Hamiltonians $\mathcal{H}$ and $\mathcal{H}_{SB}$ by adding a term:

$$\mathcal{H}_{\text{mag}} = -h \sum_{i\sigma} \sigma n_{i\sigma}.$$  \hfill (7)

Here and in the following we adopt the convention that if $\sigma$ does not appear as an index it attains the values $+1$ and $-1$ if the corresponding index is $\uparrow$ and $\downarrow$, respectively. In order to treat the density of electrons $n$ and magnetization $m$ on an equal footing, we introduce a slightly different definition for the free energy per site, to be denoted by $\varphi$. For the ferromagnet our free energy is defined as:

$$\varphi_F = -\frac{1}{\beta N} \ln \text{Tr} e^{-\beta(\mathcal{H}_{SB} + \mathcal{H}_{\text{mag}})} + \mu n + \lambda m.$$  \hfill (8)

It is given by (see also Refs.\,[4], \,[10]):

$$\varphi_F = -\frac{1}{\beta N} \sum_{k,\sigma} \ln \left[ 1 + e^{-\beta E_\sigma(k)} \right] + Ud^2 + \bar{\mu} n + \bar{\lambda} m,$$

where

$$E_\sigma(k) = q_\sigma t(k) - \sigma \bar{\lambda} - \bar{\mu},$$  \hfill (10)

with

$$t(k) = -2t(\cos k_x + \cos k_y),$$  \hfill (11)

the band structure of freely hopping electrons on a square lattice. The density $n$ and magnetization $m$ are given by: $n = n_\uparrow + n_\downarrow$ and $m = n_\uparrow - n_\downarrow$ with $n_\sigma = \langle n_{i\sigma} \rangle$. Since in principle the electrons have been integrated out in obtaining (8), $n$ and $m$ can be understood as a shorthand for the Bose fields $p_\uparrow$ and $p_\downarrow$ via the relation: $n_\sigma = p_\sigma^2 + d^2$ (which is the average of constraint (3)). The parameters $\bar{\mu}$ and $\bar{\lambda}$ are an effective chemical potential and effective magnetic field, respectively, which incorporate the Lagrange multipliers $\lambda_\sigma^{(2)}$ used to enforce the constraints (3):

$$\bar{\mu} = \mu - \frac{1}{2} \left( \lambda_\uparrow^{(2)} + \lambda_\downarrow^{(2)} \right),$$  \hfill (12)

$$\bar{\lambda} = h - \frac{1}{2} \left( \lambda_\uparrow^{(2)} - \lambda_\downarrow^{(2)} \right).$$  \hfill (13)

The Lagrange multiplier $\lambda^{(1)}$ associated with constraint (2) has disappeared because the average of this constraint must hold. In fact, both constraints are only satisfied on average in the saddle-point approximation. The band-renormalization factor $q_\sigma$ appearing in (10) is in this approximation of time- and position-independent Bose fields a function of $n, m$ and $d$ (as follows directly from (4)-(5)):

$$q_\sigma(n, m, d) \equiv \langle z^\dagger_{j\sigma} z_{i\sigma} \rangle = \frac{\sqrt{(1-n+d^2)(n+\sigma m - 2d^2) + d\sqrt{n-\sigma m - 2d^2}^2}}{(n+\sigma m) \left[ 1 - \frac{1}{2} (n+\sigma m) \right]^2}.$$  \hfill (14)

We note that if this $q_\sigma$ is rewritten as a function of $n_\uparrow, n_\downarrow$ and $d$ one exactly recovers the expression for the band renormalization in the Gutzwiller approximation (see Ref.\,[17]; our $d^2$ is called $d$ there\,[3]). This would not be true if another choice for $z_{i\sigma}$ than (3) had been made.

\footnote{In Ref.\,[4] similar renormalization factors are derived in an alternative manner.}
The sum over $k$ in (9) is over the whole Brillouin zone of the square lattice. In the limit of an infinitely large lattice, which can be treated after the approximations made, the resulting integral over the (two-dimensional) Brillouin zone can be rewritten as an (one-dimensional) integral over energy using the density of states (DOS) of freely hopping electrons. For the square lattice this DOS, $N(\varepsilon)$, is known analytically:

$$N(\varepsilon) \equiv \frac{1}{N} \sum_{k} \delta(\varepsilon - t(k)) = \begin{cases} \frac{1}{2\pi^2 t} K \left[ 1 - \left( \frac{\varepsilon}{4t} \right)^2 \right] & |\varepsilon| \leq 4t \\ 0 & |\varepsilon| > 4t \end{cases},$$

where $K(x)$ is the complete elliptic integral of the first kind [18]. Employing the DOS the free energy is:

$$\varphi_F = -\frac{1}{\beta} \sum_{\sigma} \int d\varepsilon N(\varepsilon) \ln \left[ 1 + e^{-\beta E_\sigma(\varepsilon)} \right] + U d^2 + \bar{\mu} n + \bar{\lambda} m,$$

with $E_\sigma(\varepsilon) = q_\sigma \varepsilon - \sigma \bar{\lambda} - \bar{\mu}$. Unless stated otherwise explicitly integrals over $\varepsilon$ run from $-\infty$ to $\infty$ (the relevant integration range is of course limited by (15)).

For a given interaction strength $U$, $\varphi_F$ is now given as a function of the five variables $n, m, d, \bar{\mu}$ and $\bar{\lambda}$, whereas $\mu$ and $h$ are control parameters, regulating (although not directly in this slave-boson approach) the density and magnetization. The optimal values for the five variables must be found from the three minimization conditions: $\partial \varphi_F / \partial d = 0$, $\partial \varphi_F / \partial \bar{\mu} = 0$, $\partial \varphi_F / \partial \bar{\lambda} = 0$, as well as from the two equations arising from the Legendre transform between grand potential (function of $\mu$ and $h$) and free energy (function of $n$ and $m$): $\partial \varphi_F / \partial m = h$ and $\partial \varphi_F / \partial n = \mu$.

Applying these conditions to (16) results in:

$$U = -\frac{1}{2d} \sum_{\sigma} q_{\sigma d} \bar{\varepsilon}_\sigma,$$

$$n = \sum_{\sigma} n_{\sigma},$$

$$m = \sum_{\sigma} \sigma n_{\sigma},$$

$$\bar{\lambda} = h - \sum_{\sigma} q_{\sigma m} \bar{\varepsilon}_\sigma,$$

$$\bar{\mu} = \mu - \sum_{\sigma} q_{\sigma n} \bar{\varepsilon}_\sigma,$$

where $q_{\sigma \alpha}$ denotes the first partial derivative of $q_\sigma$ with respect to $\alpha$, and we introduced the abbreviations:

$$n_{\sigma} = \int d\varepsilon N(\varepsilon) f [E_\sigma(\varepsilon)]$$

and

$$\bar{\varepsilon}_\sigma = \int d\varepsilon N(\varepsilon) \varepsilon f [E_\sigma(\varepsilon)],$$

with the Fermi-Dirac distribution, $f(E) = \left[ 1 + e^{\beta E} \right]^{-1}$. The five equations (17)–(21) need to be solved self-consistently for given $U$, $\mu$ and $h$ and the results can be inserted in (16) to obtain the corresponding free energy. In practice, we will often be
interested in calculations for a fixed density \( n \), in which case the last equation (21) does not appear (\( \mu \) disappears from the problem, however \( \bar{\mu} \) remains). Expressions for partial derivatives of \( q_\sigma \) are given in Appendix A.

The above allows to compute the free energy of three different phases: the paramagnetic phase (PM), for which \( m = 0 \) if \( h = 0 \), the strong ferromagnet (SF), for which \( m = n \) and both are non-zero even if \( h = 0 \), and the weak ferromagnet (WF), for which \( m < n \) and both are non-zero even if \( h = 0 \). In Section 3, we will obtain the lines in the \((t/U, n)\)-diagram of first-order phase transitions between these phases. In order to obtain the line of the continuous phase transition between paramagnet and ferromagnet (the ferromagnet can be either strong or weak), one needs to find where the susceptibility \( \chi \) of the paramagnet diverges. An expression for \( \chi \) is derived in Appendix B.

### 2.2 Anti-ferromagnetic Phase

For the antiferromagnetic phase we divide the square lattice in two sublattices, such that points on one sublattice have only points of the other sublattice as nearest neighbours. Furthermore, we assume a non-zero staggered magnetization \( m_s \), i.e. the magnetization is \( m_s \) on one sublattice and \( -m_s \) on the other. To be able to calculate the staggered susceptibility we add a staggered-magnetic-field term to the Hamiltonians \( \mathcal{H} \) and \( \mathcal{H}_{SB} \):

\[
\mathcal{H}_{\text{mag},s} = -\sum_{i\sigma} h_{i,s}\sigma n_{i\sigma} ,
\]

(24)

where \( h_{i,s} \) equals \( h_s \) on one sublattice and \( -h_s \) on the other. The saddle-point approximation of time- and position-independent Bose-fields on each of the two sublattices separately (introducing staggered Lagrange multipliers as well) results in a \( 2 \times 2 \) problem (for each \( \sigma \) separately, only one-electron states with \( \mathbf{k} \) and \( \mathbf{k} + \mathbf{Q} \) couple, \( \mathbf{Q} \equiv (\pi, \pi) \)) for the quasi-particle spectrum, which is easily diagonalized. Analogously to the ferromagnet, we define the “free energy” per site for the antiferromagnet as:

\[
\varphi_{AF} = -\frac{1}{\beta N} \ln \text{Tr} e^{-\beta (\mathcal{H}_{SB} + \mathcal{H}_{\text{mag},s})} + \mu n + h_s m_s .
\]

(25)

It is given by:

\[
\varphi_{AF} = -\frac{1}{\beta N} \sum_{\mathbf{k},\sigma}' \ln \left[ 1 + e^{-\beta E(\mathbf{k})} \right] + Ud^2 + \tilde{\mu} n + \tilde{\lambda}_s m_s ,
\]

(26)

where

\[
E(\mathbf{k}) = \pm \sqrt{q_s^2 l^2(\mathbf{k}) + \tilde{\lambda}_s^2} - \tilde{\mu} ,
\]

(27)

and we have again introduced an effective chemical potential \( \tilde{\mu} \) and an effective magnetic field \( \tilde{\lambda}_s \). The prime indicates that the sum over \( \mathbf{k} \) is over the magnetic Brillouin zone only \((k_x, k_y) \in [-\pi, \pi])\). The band-renormalization factor \( q_s \) is now a \( \sigma \)-independent quantity because of the staggering:

\[
q_s(n, m_s, d) \equiv \langle z_{j\sigma}^\dagger z_{i\sigma} \rangle_{AF} = z_{A\sigma} z_{B\sigma} = z_\uparrow z_\downarrow ,
\]

(28)
where
\[
\sigma = \sqrt{(1 - n + d^2)(n + \sigma m_s - 2d^2) + d\sqrt{n - \sigma m_s - 2d^2}} \sqrt{(n + \sigma m_s)(1 - \frac{n + \sigma m_s}{2})}. 
\] (29)

As for the ferromagnet, the free energy can be expressed as an integral over the DOS of freely hopping electrons, \( N(\varepsilon) \):
\[
\varphi_{AF} = -\frac{1}{\beta} \int d\varepsilon N(\varepsilon) \ln \left[ 1 + e^{-\beta E(\varepsilon)} \right] + Ud^2 + \tilde{\mu} n + \tilde{\lambda}_s m_s . 
\] (30)

For convenience we restrict ourselves to densities \( n \leq 1 \); in that case only the negative square root in (27) is relevant and we have in (30):
\[
E(\varepsilon) = -\sqrt{q^2\varepsilon^2 + \lambda_s^2} - \tilde{\mu} . 
\] (31)

The consistency equations for the antiferromagnet are obtained in the same way as for the ferromagnet and read:
\[
U = \frac{qsd}{2d^2} , 
\] (32)
\[
n = \int d\varepsilon N(\varepsilon)f[E(\varepsilon)] , 
\] (33)
\[
m_s = \tilde{\lambda}_s \int d\varepsilon \frac{N(\varepsilon)f[E(\varepsilon)]}{\sqrt{q^2\varepsilon^2 + \lambda_s^2}} , 
\] (34)
\[
\tilde{\lambda}_s = h_s + qsm_s\bar{\varepsilon} , 
\] (35)
\[
\tilde{\mu} = \mu + qsn\bar{\varepsilon} , 
\] (36)

where we have defined:
\[
\bar{\varepsilon} = q_s \int d\varepsilon \frac{N(\varepsilon)\varepsilon^2f[E(\varepsilon)]}{\sqrt{q_s^2\varepsilon^2 + \tilde{\lambda}_s^2}} . 
\] (37)

Expressions for partial derivatives \( q_{sa} \) of \( q_s \) are given in Appendix C. \( \varphi_{AF} \) is a function of the five variables \( n, m_s, d, \tilde{\mu} \) and \( \tilde{\lambda}_s \), whereas \( \mu \) and \( h_s \) are control parameters. Calculating \( \varphi_{AF} \) for fixed \( U/t \) and \( n \), means that the last consistency equation (36) becomes irrelevant again and the four remaining variables must be found self-consistently from the four remaining consistency equations. To compute the free energy the staggered field \( h_s \) is taken to be zero. This free energy may be compared to the free energies of the three phases discussed in the previous subsection and lines of first-order transitions in the \((t/U, n)\)-plane may be found (see Section 3). We note that the equations for the paramagnet can also be found from the above equations for the antiferromagnet by putting \( m_s = 0 \) if \( h_s = 0 \) (then also \( \tilde{\lambda}_s = 0 \)). In order to find the transition line for the continuous phase transition between antiferromagnet and paramagnet an expression for the staggered susceptibility \( \chi_s \) is derived in Appendix D.
2.3 Spiral Phase

To obtain the spiral phase the magnetization vector is assumed to vary in space as:

\[ \mathbf{m}_i = m(\cos(\mathbf{q} \cdot \mathbf{R}_i), \sin(\mathbf{q} \cdot \mathbf{R}_i), 0) . \]  

(38)

In Ref.[16], the spin-rotation invariant formulation is used to compute the free energy \( \varphi_{sp} \) for this phase. For details of this calculation we refer to Refs.[8, 16], here we suffice by quoting the result (in our notation):

\[ \varphi_{sp} = -\frac{1}{\beta N} \sum_{k,\nu} \ln \left[ 1 + e^{-\beta E_{q,\nu}(k)} \right] + U d^2 + \tilde{\mu} n - \lambda^{(2)} m . \]  

(39)

where

\[ E_{q,\nu}(k) = \left( z_+^2 + z_-^2 \right) \left[ \frac{t(k) + t(k + \mathbf{q})}{2} \right] - \tilde{\mu} + \]

\[ + \nu \left\{ \left( z_+^2 - z_-^2 \right)^2 \left[ \frac{t(k) - t(k + \mathbf{q})}{2} \right]^2 + z_+ z_- [t(k) + t(k + \mathbf{q})] + \lambda^{(2)} \right\}^{\frac{1}{2}} , \]  

(40)

with \( \nu = \pm 1 \). The parameters \( z_\pm \) are functions of \( n, m \) and \( d \); in terms of the \( z_\sigma \) (formula (29) with \( m_s \) replaced by \( m \)) they are given by:

\[ z_\pm = \frac{1}{2} \left( z^\uparrow \pm z^\downarrow \right) . \]  

(41)

The parameter \( \tilde{\mu} = \mu - \lambda^{(2)}_0 \) is again an effective chemical potential, whereas \( \lambda^{(2)}_0 \) and \( \lambda^{(2)} \) are the Lagrange multipliers arising from the constraint (3) when made spin-rotation invariant.\(^3\) We did not include any explicit magnetic field in the Hamiltonian in studying the spiral phases. One may verify that for \( \mathbf{q} = (0, 0) \) and \( \mathbf{q} = (\pi, \pi) \) (10) reduces to the expressions (10) and (27) for the ferromagnet and antiferromagnet, respectively. In terms of the \( z_\pm \) the band-renormalization factors are given by \( q_\sigma = (z_+ + \sigma z_-)^2 \) and \( q_s = z_+^2 - z_-^2 \).

For the spiral phase we do not give the consistency equations like we did for the ferromagnet and antiferromagnet, since we are only aiming at a simple phase diagram which does not include the spiral phases. Moreover, the consistency equations and free energy cannot be expressed as one-dimensional integrals over a density of states because of the spiraling vector \( \mathbf{q} \) involved. Therefore, the consistency equations need to be solved numerically on a finite lattice. The regions in the phase diagram where spiral phases dominate the simple magnetic phases were calculated in Refs.[16] and [19]. In this paper, we will only use the expressions above to derive a formula within SBMF approximation for the helicity modulus (or: spin stiffness) and effective hopping parameter in Section 4.

3 Magnetic Phase Diagram

We compute, in SBMF approximation, the complete (i.e. all first order and continuous phase transitions are included) ground-state magnetic phase diagram for the

\[^3\]In the spin-rotation invariant formulation, constraint (3) gives rise to a scalar Lagrange multiplier \( \lambda^{(2)}_0 \) as well as a vector Lagrange multiplier \( \tilde{\mathbf{\lambda}}^{(2)} \). For a spiral phase the latter results in another scalar \( \lambda^{(2)} = |\tilde{\mathbf{\lambda}}^{(2)}| \) because it must show the same spatial variation as \( \mathbf{m} \) in (38).
Hubbard model on a square lattice allowing for the four simple magnetic phases, paramagnet (PM), weak ferromagnet (WF), strong ferromagnet (SF) and antiferromagnet (AF). In their original paper, Kotliar and Ruckenstein \[4\] only calculated the lines where the PM becomes unstable towards ferromagnetic or antiferromagnetic ordering (continuous transitions), whereas Evans \[10\] also included some first-order transitions, but not all, so that an incomplete picture emerged.

First, the regions in the \((4t/U, n)\)-plane where ferromagnetism (either WF or SF) and antiferromagnetism can occur are determined, by calculating the lines where the homogeneous and staggered susceptibilities, \(\chi\) and \(\chi_s\), of the PM diverge. In Appendices B and D expressions for \(\chi\) and \(\chi_s\) are derived. The condition that the denominator in these expressions vanishes (generalized Stoner criterion) provides an additional equation to be solved in conjunction with the consistency equations for the PM (see Section 2.1). In this way, for fixed \(n\), the additional equation fixes the (critical) \(U/t\) value for which the susceptibility diverges. The resulting lines are displayed in Figure 1(a) and agree with previously published results \[4, 10\].

Now, using the formulae in Sections 2.1 and 2.2 all first order phase transition lines in the \((4t/U, n)\)-diagram are computed. Since no susceptibilities are required, \(h\) and \(h_s\) are taken to be zero. In principle, for each of the four phases for fixed values of \(U/t\) and \(n\) the energy is found by solving the consistency equations simultaneously\(^4\). For the SF and PM this problem simplifies somewhat: for the SF the set of equations (17)-(20) is reduced by one (since \(m = n\)) and for the PM we have \(m = 0\). For each pair of phases one then finds a line in the \((4t/U, n)\)-plane where the two energies are equal. The results of such calculations are displayed in Fig. 1(a). In principle there are six such lines, but the first order PM/AF transition line coincides with the continuous PM/AF transition. Note however that the continuous PM/F transition and the first order PM/WF transition differ.

Taking into account all four phases, the phase diagram of the Hubbard model on a square lattice in SBMF approximation of Figure 1(b) emerges, in which all interrupted lines denote first-order transitions and the full line a continuous (PM/AF) transition. We now discuss the phase diagram in comparison with the same phase diagram as obtained in the Hartree-Fock approximation (HFA) and in comparison with previously published SBMF results.

The corresponding, i.e., allowing for the same four phases, phase diagram to Fig.1(b) in the HFA is shown in Figure 1(c). A similar diagram was given previously in three dimensions by Penn \[21\] and in two dimensions by Hirsch \[22\], but in the latter the non-monotonous behaviour of the F/AF transition line was missed and the region of WF was not determined. Long has given the PM/F/AF phase diagram in HFA using a constant density of states; in that case no extremum in the F/AF transition occurs \[23\]. Another surprising feature of Fig.1(c), besides the maximum in the F/AF line, is the fact that the WF/SF transition line is found to oscillate slightly around the line of the continuous P/F line. The difference in these curves is very small, but we have ascertained that it is not due to numerical inaccuracies. Thermodynamically such behaviour is allowed; it only means that along the P/F

---

\(^4\)Using the analytically known density of states \(15\) this may be conveniently done with the program MATHEMATICA \[20\]. Some care is required in integrating through the logarithmic singularity of \(N(\varepsilon)\) in \(\varepsilon = 0\).
boundary the transition is sometimes continuous and sometimes first order. In comparing Fig.1(b) and Fig.1(c) it should be noted that they are topologically the same, but that because of the difference in scale on both the density and 4t/U axes, the SBMF has reduced the magnetically ordered regions considerably with respect to the HFA. Furthermore, the region where WF dominates has grown at the expense of the SF phase. In Table I, we list the location of the “tripod” points (i.e., points where three phases meet; the AF/SF/WF and PM/SF/WF points are triple points, i.e., points where three first-order transitions meet), as well as the renormalization factor obtained in going from the HFA to the SBMF approximation. Globally speaking this factor is about 3 for the hole density δ and also about 3 for t/U (if the ferromagnetic region is considered as a whole). Since the HFA overestimates the importance of magnetic ordering [23], the SBMF approximation is clearly an improvement. The critical hole density above which antiferromagnetism cannot occur is determined by the continuous PM/AF transition and is given by $\delta_{c}^{AF} = 0.21$ in SBMF. More interestingly, the critical hole density above which ferromagnetism cannot occur is in SBMF determined by the first order PM/SF transition and given by exactly $\delta_{c}^{F} = 1/3$, as a simple argument can show (see e.g. Ref.[19]). The latter value agrees very well with the result $\delta_{c}^{F} = 0.29$ obtained from calculations using a variational wave function [24]. Remarkably, also high-temperature series expansions for the Hubbard model find for $U/t \to \infty$ a value of about 0.33, below which ferromagnetic nearest-neighbour correlations occur [25], and a value “near 3/11” ($\simeq 0.27$), below which a strong separation of energy scales for spin and translational degrees of freedom is observed [26]. Although these features in the high-temperature series expansions appear to be temperature independent over a wide temperature range, extrapolation to $T = 0$ is cumbersome in such expansions [27]. We also note that the $\chi^{-1} = 0$ line is nowhere in the diagram a phase boundary; therefore the continuous PM/F transition, in this approximation and contrary to the HFA result, is preempted by first order PM/WF or PM/SF transitions.

A calculation of the phase diagram similar to ours was previously performed by Evans [10]. However, the more cumbersome PM/WF and AF/WF first order transitions were not computed and for the WF/SF transition only the limit $m = n$ and $d = 0$ in the WF was taken. The latter determination turns out only to give an upper bound (in $t/U$, for fixed $n$) for the WF/SF first-order transition computed by comparing energies, as it should. As a result the final phase diagram of Ref.[10] is obtained by removing from Fig.1(a) the PM/WF and AF/WF lines and replacing the WF/SF line by one extending from (0.15,0.0) to (0.0,0.38) in the (4t/U, δ)-plane ($\delta = 1 - n$). Evans then appears to call WF only the tiny, triangle-shaped, region at the center of our WF region (although this is not very clear from Fig.1 in Ref.[10]). This assignment, however, is thermodynamically not justified since two of the boundaries then correspond to PM/SF and PM/AF transitions. Also the third boundary in that case (PM/F) is not a boundary for the WF region as computed by us.

To conclude the discussion of the phase diagram in Fig.1, we stress that the actual ground-state phase diagram of the Hubbard model, even when constructed within either the HF or SBMF approximation, will also have to include inhomogeneous phases like domain walls and spiral phases. For instance, it was shown
within the SBMF approximation that spiral phases supersede the antiferromagnet immediately when going off half-filling and also the ferromagnetic phases shrink somewhat in favour of certain spiral phases \[16, 19\]. Our detailed determination of the simple phase diagram only serves to study the consequences of the SBMF approximation when compared with the HFA.

4 Helicity Modulus and Effective Hopping

A crucial quantity in the study of quantum-ordered states is the helicity modulus, which is the stiffness associated with a twist of the order parameter, or, equivalently, with phase fluctuations of a complex order parameter. For the attractive Hubbard model, which exhibits superconducting or superfluid order, the helicity modulus corresponds to the superfluid density, whereas for the repulsive Hubbard model it is the spin stiffness of the AF ordered phase at half-filling. In previous papers, the helicity modulus, denoted by \(\rho_s\), was calculated for the 2D Hubbard model both in the HFA as well as by variational Monte Carlo methods \[11, 12\]. Also a comparison with exact diagonalization and Quantum Monte Carlo results was made, showing that the HFA renders quantitatively reasonable results for \(\rho_s\) \[13\]. For the repulsive Hubbard model this could only be shown at half-filling. Since we have already seen that the SBMF approximation is an improvement over the HFA, it is of interest to see what it will give for \(\rho_s\). In this section, we first derive an expression for \(\rho_s\) within the SBMF approximation and use it to compute \(\rho_s\). Then the connection between \(\rho_s\) and the effective hopping parameter is discussed, leading to calculations of the effective hopping both at half-filling and off half-filling. The SBMF results are compared to results from the HFA and Quantum Monte Carlo results.

To obtain \(\rho_s\), we can make use of the results for the spiral phase in Section 2.3. In the AF phase the order parameter is the staggered magnetization. This can be viewed as a spiral phase with spiral vector \(q = Q \equiv (\pi, \pi)\). A small twist in the AF order parameter then corresponds to a spiral vector which deviates slightly from \(Q\):

\[
q = (\pi, \pi) - \tilde{q}.
\]

The helicity modulus \(\rho_s\) is given by:

\[
\rho_s = \lim_{\tilde{q} \to 0} \frac{\varphi(\tilde{q}) - \varphi(0)}{\frac{1}{2}\tilde{q}^2},
\]

with the free energy per site \(\varphi\) given by \[39\] and where \(\tilde{q}\) is the modulus of \(\tilde{q}\). To facilitate the computation it is advantageous to perform a further manipulation. Since the spectrum is periodic in reciprocal space and we are going to integrate over the full Brillouin zone, it is allowed to shift the spectrum over \(\frac{1}{2}\tilde{q}\), so that \[40\] becomes (if in turn we rename \(\frac{1}{2}\tilde{q}\), for notational convenience, to \(q\)):

\[
E_{q,\nu}(k) = \left(z_+^2 + z_-^2\right) \left[\frac{t(k+q)-t(k-q)}{2}\right] - \bar{\mu} + \\
+ \nu \left\{ \left(z_+^2 - z_-^2\right) \left[\frac{t(k+q)+t(k-q)}{2}\right]^2 + \left[ z_+z_- [t(k+q) - t(k-q)] + \lambda(2) \right] \right\}^\frac{1}{2}.
\]
with $\nu = \pm 1$. After this manipulation, the occurring sum $t(k + q) + t(k - q)$ is even in the small parameter $q (= |q|)$ and the difference is odd. The same is not true for the small parameter $\tilde{q}$ in the occurring sum and difference $t(k) \pm t(k + Q - \tilde{q})$ in (10). In this notation, $\rho_s$ is given by:

$$\rho_s = \lim_{q \to 0} \frac{\varphi(q) - \varphi(0)}{2q^2}, \quad (45)$$

If we now restrict to ground-state properties ($T = 0$) and densities less than half-filling ($n < 1$), we only need to expand the $\nu = -1$-branch for small $q$ (and integrate over the Brillouin zone (BZ)) to obtain $\varphi(q) - \varphi(0)$ to order $q^2$. We find (taking $q = (q, 0)$ for convenience) that the term proportional to $q$ vanishes after integrating over BZ, and that $\rho_s$ is given by:

$$\rho_s = -\frac{tq_s^2}{N_s} \sum_k \left[ \frac{t(k)\cos(kx)}{2E(k)} + \frac{4tz^2z^2t^2(k)\sin^2(kx)}{E^3(k)} \right] \quad (46)$$

with

$$E(k) = \sqrt{q_s^2t^2(k) + \lambda^2}, \quad (47)$$

and the band renormalization $q_s$ is:

$$q_s = z_+^2 - z_-^2. \quad (48)$$

We have omitted the superscript (2) on $\lambda$. We remark that if the above shift in the BZ is not performed, a much longer expression for $\rho_s$ results; the expression is equivalent to (46), but this is not trivial. We further note that the $T = 0$ HFA result of Ref.[11] is recovered by omitting the second term in the BZ sum and putting $q_s$ equal to 1.

In order to compute $\rho_s$ for fixed density $n$, according to Section 2.2, the following set of equations needs to be solved self-consistently (for $T = 0$ and $\hbar_s = 0$; cf. (32)-(35)):

$$m_s = 2\tilde{\lambda} \int_\mu^4 \frac{\mathcal{N}(\varepsilon)}{(\varepsilon^2 + \tilde{\lambda}^2)^{1/2}}, \quad (49)$$

$$\tilde{\lambda} = \frac{2}{q_s} q_{sma} \int_\mu^4 \frac{\mathcal{N}(\varepsilon)\varepsilon^2}{(\varepsilon^2 + \tilde{\lambda}^2)^{1/2}}, \quad (50)$$

$$U = \frac{q_{sd}}{d} \int_\mu^4 d\varepsilon \frac{\mathcal{N}(\varepsilon)\varepsilon^2}{(\varepsilon^2 + \tilde{\lambda}^2)^{1/2}}, \quad (51)$$

where $\tilde{\lambda} = \lambda/q_s$ and $\tilde{\mu}$ is determined by the fixed $n$:

$$n = 2 \int_\mu^4 \frac{\mathcal{N}(\varepsilon)}{\varepsilon}, \quad (52)$$

In terms of the parameters of Section 2.2, we have $\tilde{\mu} = \sqrt{\tilde{\mu}^2 - \tilde{\lambda}^2}/q_s$ ($\tilde{\lambda}_s$ is called $\lambda$ here). The band renormalization $q_s$ is given by (28)-(29). In terms of an integral
over the DOS, the energy of the AF state (per site) and the spin stiffness $\rho_s$ are given by:

$$e_{AF} = -2q_s \int_{\mu}^{4} d\varepsilon \sqrt{\varepsilon^2 + \lambda^2} + Ud^2 + \bar{\lambda}q_sm_s$$  \quad (53)$$

$$\rho_s = \frac{q_s}{4} \int_{\mu}^{4} d\varepsilon \frac{\mathcal{N}_v(\varepsilon)\varepsilon^2}{(\varepsilon^2 + \bar{\lambda}^2)^{3/2}} - \frac{z_+^2 z_-^2}{q_s} \int_{\mu}^{4} d\varepsilon \frac{\mathcal{N}_v(\varepsilon)\varepsilon^2}{(\varepsilon^2 + \bar{\lambda}^2)^{3/2}}$$  \quad (54)$$

where $\mathcal{N}_v(\varepsilon)$ is the weighted density of states:

$$\mathcal{N}_v(\varepsilon) \equiv \frac{1}{N} \sum_{\mathbf{k}} |\nabla t(\mathbf{k})|^2 \delta(\varepsilon - t(\mathbf{k})),$$  \quad (55)$$

which for a square lattice can be calculated analytically (see Ref. [28]):

$$\mathcal{N}_v(\varepsilon) = \frac{8t}{\pi^2} \left\{ E \left[ 1 - \left( \frac{\varepsilon}{4t} \right)^2 \right] - \left( \frac{\varepsilon}{4t} \right)^2 K \left[ 1 - \left( \frac{\varepsilon}{4t} \right)^2 \right] \right\},$$  \quad (56)$$

for $|\varepsilon| \leq 4t$ and zero otherwise. $K(x)$ and $E(x)$ are the complete elliptic integrals of the first and second kind, respectively. We remark that using the weighted density of states the finite-temperature result for $\rho_s$ obtained in the HFA [11] can also be written as an integral over energy.

Since only at half-filling the AF phase is the ground-state, we first restrict ourselves to this case: $n = 1$ ($\bar{\mu} = 0$). In Table II, self-consistent parameters are given for various $U/t$; the corresponding energy $e_{AF}$ and band renormalization $q_s$ are also given. These results agree with those published previously by Hasegawa [29]. In particular, we note that $q_s$ never deviates from 1 by more than 5%, implying that slave bosons at half-filling renormalize the Hartree-Fock results only by a small amount. As concerns $\rho_s$, for the case of half-filling the integral containing $\mathcal{N}_v(\varepsilon)$ plays no role since for $n = 1$ we have $z_- = 0$ (as is easily verified from (29) and (41)). In Table III and Figure 2, we compare the results for $\rho_s$ obtained in the SBMF, with those obtained previously using the HFA and using variational Monte Carlo calculations with an (antiferromagnetic) Gutzwiller wave function (GWVMC) [11]. The fact that slave bosons only renormalize the HF results a little bit is reflected in the fact that the SBMF and HF results never differ by more than 7%. Note however that the SBMF result is always larger (except for very small $U/t$, $U/t < 2.5$), whereas $q_s$, which enters as a factor in (54), is smaller than 1. The direct effect of $q_s$ is more than compensated by a renormalized (smaller) value of the antiferromagnetic gap $\lambda = \bar{\lambda}q_s$. A further observation from Table III and Fig.2 is that the SBMF results almost coincide with the GWVMC results. The difference between the results is an indication of the difference between the Gutzwiller approximation (which is equivalent to the present SBMF approximation, see the introduction) and the Gutzwiller wave function. Although these are not identical [3], the difference for the spin stiffness is not big, as shown in Fig.2. Therefore the tedious variational Monte Carlo calculations for $\rho_s$ can be replaced by the above set of equations which are exact (within the SBMF) and easy to solve.

On very general grounds it can be derived that the helicity modulus (spin stiffness for positive $U$ and superfluid weight for negative $U$) comprises of a “direct” part
proportional to the average kinetic energy $\langle T \rangle$ and a part related to the current-current correlation function $\Lambda_{xx}$ [30]. The HFA effectively neglects the $\Lambda_{xx}$-part, whereas GWVMC calculations find only a negligible correction to the kinetic part $-\frac{1}{2} \langle T \rangle$ [11]. Since in formula (46) the first term is exactly $-\frac{1}{2} \langle T \rangle$ in the SBMF approximation and at half-filling the second term equals zero, we can conclude that also the SBMF approximation only gives the kinetic part of $\rho_s$. In Ref.[13] it was estimated (by comparing to appropriate exact diagonalization calculations and Quantum Monte Carlo (QMC) calculations) that the HFA overestimates $\rho_s$ at half-filling by 68, 40, 38 and 36 % for $U/t = 4, 8, 10$ and 20, respectively. However, if one compares the kinetic energy found in the HF and SBMF approximations with QMC calculations for $n = 1$ (The latter are obtained from Ref.[32]), one concludes that the approximations perform very satisfactorily. This is illustrated in Figure 3, where we plot the effective hopping integral $t_{\text{eff}}$, defined by normalizing the average kinetic energy for interaction constant $U$ with that for $U = 0$:

$$\frac{t_{\text{eff}}}{t} = \frac{\langle c_i^\dagger c_j^\sigma + c_j^\dagger c_i^\sigma \rangle U}{\langle c_i^\dagger c_j^\sigma + c_j^\dagger c_i^\sigma \rangle U = 0}.$$  

(57)

The denominator is easily evaluated as the energy of the PM phase in the HFA, since for $U = 0$ the HFA is exact and there is no potential energy. The QMC data is taken at sufficiently low temperature ($\beta t = 16$) for this comparison with $T = 0$ results to be meaningful. We note that a similar comparison of SBMF and QMC data was made in Ref.[31]; in that paper the SBMF approach was formulated as a 14-dimensional optimization problem. By comparing their Figure 2(b) with our Fig.3, the results from our simple formula (54) are found to be the same. A surprising feature of Fig.3 is perhaps not so much that the SBMF results approximate the QMC results so well, but that the HFA results do the same already.

We now discuss the off-half-filling case; since off half-filling their exists a spiraling vector $q_0$ for which the spiral phase has lower energy than the AF phase, we cannot call $\rho_s$ as given by (54) the stiffness of the ground state anymore. Instead, the expression (54) has the interpretation of the stiffness of the AF phase with respect to a small deviation from spiraling vector $(\pi, \pi)$. In order to compute the stiffness of the ground state one would have to perturb the spiral phase with vector $q_0$, but this is beyond the scope of the present paper. Here we only investigate how well the effective hopping (or, equivalently, the kinetic energy) of the two-dimensional Hubbard model off half-filling is described by the first term in (54). In Figure 4(a), we compare $t_{\text{eff}}/t$ obtained from Hartree-Fock and SBMF approximations (for $T = 0$) with low-temperature ($\beta t = 6$) QMC data (The latter are obtained from Ref.[33]). The results are displayed as a function of density $n$ for the one value of $U/t (=4)$ for which there are QMC data available. From the phase diagrams in Fig.1 it is clear that both in the HFA and SBMF approximation an AF/PM transition occurs for some critical density $n_c$ ($n_c = 0.86$ in SBMF and $n_c = 0.76$ in HFA for $U/t = 4$, the former is not showing in Fig.1(a)). Below $n_c$ (paramagnetic phase), $t_{\text{eff}}/t$ equals 1 in the HFA and equals the band renormalization $q$ ($=q_\uparrow = q_\downarrow$) in the SBMF approximation. Clearly the SBMF approach

\footnote{If the restricted set of four phases is considered as before.}
is a significant improvement over the HFA; the agreement with the QMC data is less good in the density interval just off half-filling. This is most probably caused by the fact that for these densities the assumed (antiferromagnetic) phase in the SBMF approach is not the correct one. The same remark concerning Ref. [31] as made above for $n = 1$ is appropriate here. Finally, in Figure 4(b), we also show the results for the effective hopping integral for a few other values of $U/t$, for which no QMC data are available. The corresponding HFA curves are not shown, but the behaviour is similar as for $U/t = 4$: at half-filling $t_{\text{eff}}/t$ is somewhat below the SBMF result and rises to 1 in going off half-filling. The densities below which $t_{\text{eff}}/t$ equals 1 can be read off from Fig.1(c). We note that in Fig.4(b) the non-differentiability at $n_c$ (which is close to 0.8 for $U/t = 8, 12, 16$, as can be seen in Fig.1(a) and (b)) is less pronounced for $U/t = 8, 12, 16$ than it is for $U/t = 4$.

5 Discussion and Conclusions

Above we have given a detailed account of calculations within the slave-boson mean-field (SBMF) approximation for the repulsive Hubbard model on a square lattice. We have focused on the phase diagram, a particular response function, the helicity modulus $\rho_s$, and the related effective hopping integral. All calculations can be expressed in terms of a set of integral equations with one-dimensional integrals over energy containing a density of states, which is known analytically for the square lattice. These equations are solved self-consistently.

If for the $(t/U, n)$ phase diagram we restrict to simple magnetic phases, the SBMF approach is found to reduce the magnetically ordered regions with respect to the Hartree-Fock approximation (HFA). Along the density axis the reduction is roughly a factor of 3, whereas along the $t/U$-axis the reduction of the ferromagnetic region (weak- and strong ferromagnetism together) is also a factor of 3. In the SBMF approach the portion of weak ferromagnetism grows at the expense of the strong-ferromagnetism portion when compared to the HFA. The present SBMF phase diagram is more likely to be a good starting point for more sophisticated approaches to the phase diagram than is the HFA phase diagram, because in an infinite number of dimensions the SBMF approach becomes exact (see the introduction). On the other hand, it is seen that the SBMF approach is not qualitatively different from the HFA, but rather a renormalized form of HFA.

The new quantity that we obtain within the SBMF approach is the helicity modulus $\rho_s$. At half-filling, the results for $\rho_s$ practically coincide with those obtained using variational Monte Carlo calculations with a Gutzwiller wave function and are generally somewhat larger (about 5%) than those obtained in the HFA. The exact results are estimated to be smaller than the HFA results. This discrepancy is due to the neglect within the SBMF approach (as in the HFA) of the current-current correlation part of $\rho_s$. The remaining kinetic part of $\rho_s$ agrees very well with Quantum Monte Carlo (QMC) calculations of the kinetic energy or effective hopping integral. Also off half-filling, where our expression for $\rho_s$ no longer has the interpretation of helicity modulus of the ground state, it is found to represent the effective hopping much better than the HFA.
A number of extensions of the present work is possible. Most of the extensions discussed below have already been performed within the HFA and since the SBMF approach turns out to be a renormalized form of the HFA, the qualitative effect of such expansions on the present SBMF results can be predicted. A possible sequel to the present work (which was not attempted before for the HFA) is the calculation of the helicity modulus for the spiral or domain-wall phases, which supersede the AF ground state that one has at half-filling and which is the starting point for our calculated helicity modulus. Another extension is to introduce a homogeneous magnetic field $h$ in the AF phase at half-filling. Using the well-known mapping between repulsive and attractive Hubbard models (see e.g. Ref.[11]) the corresponding expression for $\rho_s$ than equals the superfluid density of the attractive ($U < 0$) Hubbard model off half-filling (without a magnetic field). A final straightforward but tedious extension of the present results is to allow for finite temperatures. The formalism set up above is perfectly capable of dealing with this more general case, but the calculations become somewhat more tedious than for $T = 0$.

Acknowledgments

We acknowledge discussions with J.M.J. van Leeuwen, J. Zaanen, and M.L. Horbach on various aspects of the work presented in this paper.
Appendix A: Band-renormalization factor $q_{\sigma}$

In this appendix expressions for partial derivatives of the band-renormalization factor $q_{\sigma}$ for the ferromagnet are given. The formula for $q_{\sigma}$, which is a function of density $n$, magnetization $m$, and density of doubly occupied sites $d^2$, is repeated here (see (14)):

$$q_{\sigma}(n, m, d) \equiv \langle z_{j\sigma}^\dagger z_{i\sigma} \rangle = \frac{\sqrt{(1 - n + d^2)(n + \sigma m - 2d^2) + d\sqrt{n - \sigma m - 2d^2}}}{(n + \sigma m)[1 - \frac{1}{2}(n + \sigma m)]}.$$

(A.1)

For $n$, $m$ and $d$ in the physically relevant range (e.g., $m$ should be less or equal than $n$ and $d^2$ should be less or equal than $\frac{1}{2}n$) $q_{\sigma}$ attains values between 0 and 1, so the free electron bands are narrowed in the SBMF approximation.

First partial derivatives $q_{\sigma n}$, $q_{\sigma m}$ and $q_{\sigma d}$ with respect to $n$, $m$ and $d$, respectively, are:

$$q_{\sigma n} = \frac{N_{\sigma}}{D_{\sigma}} \left[ \frac{e}{r_{\sigma}} - \frac{r_{\sigma}}{e} + \frac{d}{r_{\sigma}} \right] - \frac{N_{\sigma}^2}{D_{\sigma}^2} \left( 1 - n - \sigma m \right)$$

(A.2)

$$q_{\sigma m} = \sigma \frac{N_{\sigma}}{D_{\sigma}} \left[ \frac{e}{r_{\sigma}} - \frac{d}{r_{\sigma}} \right] - \sigma \frac{N_{\sigma}^2}{D_{\sigma}^2} \left( 1 - n - \sigma m \right)$$

(A.3)

$$q_{\sigma d} = 2d \frac{N_{\sigma}}{D_{\sigma}} \left[ \frac{r_{\sigma}}{e} - \frac{2e}{r_{\sigma}} + \frac{r_{\sigma}}{d} - \frac{2d}{r_{\sigma}} \right],$$

(A.4)

where we have introduced the abbreviations:

$$N_{\sigma} = \sqrt{(1 - n + d^2)(n + \sigma m - 2d^2) + d\sqrt{n - \sigma m - 2d^2}}$$

(A.5)

$$D_{\sigma} = n + \sigma m - \frac{1}{2}(n + \sigma m)^2$$

(A.6)

$$e = \sqrt{1 - n + d^2}$$

(A.7)

$$r_{\sigma} = \sqrt{n + \sigma m - 2d^2}$$

(A.8)

To determine where the susceptibility diverges (see Appendix B), we also require $q_{mm}$, the second derivative of $q_{\sigma}$ with respect to $m$ calculated at $m = 0$ (which is independent of $\sigma$):

$$q_{mm} = \frac{N_{\sigma}^2}{D_{\sigma}^2} \left[ 1 + \frac{2(1 - n)^2}{D_{\sigma}} \right] - \frac{2(1 - n)^2}{D_{\sigma}^2} - \frac{2cd}{(n - 2d^2)D_{\sigma}},$$

(A.9)

with

$$N_{0} = \sqrt{n - 2d^2} \left( \sqrt{1 - n + d^2} + d \right)$$

(A.10)

$$D_{0} = n(1 - n/2).$$

(A.11)
Appendix B: Homogeneous magnetic susceptibility for paramagnet

In this appendix we derive a formula for the homogeneous magnetic susceptibility $\chi$ in the paramagnetic phase:

$$\chi \equiv \left( \frac{\partial m}{\partial h} \right)_{h=0}. \tag{B.1}$$

The derivation proceeds as follows: in the paramagnet, we have $m = 0$ if $h = 0$ in the equations (17)–(21) of Section 2.1. Then also $\lambda = 0$. The solutions of the consistency equations of the remaining variables we call $n_0$, $d_0$ and $\bar{\mu}_0$. Now we apply an infinitesimal magnetic field $\delta h$. Then $m$ and $\lambda$ will acquire small non-zero values $\delta m$ and $\delta \lambda$ and the other quantities will deviate slightly from their values for $h = 0$, because all are coupled through (17)–(21). If we now work at a fixed density (i.e., $n$ is not allowed to deviate from $n_0$ and equation (21) becomes irrelevant), we have four equations containing five small quantities. From these the required ratio $\frac{\delta m}{\delta h}$ is obtained. Working out this procedure, by expanding all equations to first order in the small quantities, it turns out (perhaps not surprisingly) that the equations for $\delta \bar{\mu}$ and $\delta d$ decouple from those for $\delta m$, $\delta \lambda$ and $\delta h$. Here we give the equations for the latter three quantities for the case $T = 0$ (for which the derivative of the Fermi-Dirac distribution is a convenient delta-function):

$$\delta m = a \delta m + \chi_0 \delta \lambda, \tag{B.2}$$

$$\delta \lambda = \delta h + b \delta m + a \delta \lambda, \tag{B.3}$$

where we have introduced the following notation:

$$\chi_0 = \frac{2N_F}{q}, \tag{B.4}$$

$$a = -\frac{2N_F q_m \bar{\mu}_0}{q^2}, \tag{B.5}$$

$$b = -2q_{mm} \bar{\varepsilon}_0 + \frac{2N_F q_m^2 \bar{\mu}_0^2}{q^3}, \tag{B.6}$$

with

$$N_F = N(\bar{\mu}_0/q), \tag{B.7}$$

$$\bar{\varepsilon}_0 = \int_{-\infty}^{\bar{\mu}_0/q} d\varepsilon N(\varepsilon) \varepsilon \tag{B.8}$$

and $q$ and $q_m$ are the functions $q_\sigma$ and $q_{\sigma m}$ taken at $m = 0$ (see Appendix A). Solving (B.2) and (B.3) for $\chi$ finally gives the required formula for the susceptibility:

$$\chi = \frac{\chi_0}{(1 - a)^2 - b \chi_0}. \tag{B.9}$$

A similar result was given in Ref.[10], although there is a factor of 2 difference in the $\bar{\varepsilon}_0$-term in (B.6).
Appendix C: Band-renormalization factor $q_s$

In this appendix expressions for partial derivatives of the band-renormalization factor $q_s$ for the antiferromagnet are given. The formula for $q_s$, which is a function of density $n$, staggered magnetization parameter $m_s$, and density of doubly occupied sites $d^2$, is repeated here (cf. (28)-(29)):

$$q_s(n, m_s, d) = z(n, m_s, d) z(n, -m_s, d), \quad (C.1)$$

where

$$z(n, m_s, d) = \frac{\sqrt{(1 - n + d^2)(n + m_s - 2d^2) + d\sqrt{n - m_s - 2d^2}}}{\sqrt{(n + m_s)(1 - \frac{n + m_s}{2})}}. \quad (C.2)$$

Introducing the abbreviations $N_\pm$ and the partial derivative of $z$ with respect to $m_s$:

$$N_\pm = \sqrt{(n \pm m_s)(1 - \frac{n \pm m_s}{2})}, \quad (C.3)$$

$$\frac{\partial z}{\partial m_s} = \frac{1}{2N_+} \left\{ \frac{\sqrt{1 - n + d^2}}{n + m_s - 2d^2} - \frac{d}{\sqrt{n - m_s - 2d^2}} - \frac{z(n, m_s, d)}{N_+} [1 - n - m_s] \right\} \quad (C.4)$$

the first partial derivatives with respect to $m_s$ and $d$ are (since we always work at fixed density, the derivative with respect to $n$ is not needed):

$$q_{s m_s} = z(n, -m_s, d) \frac{\partial z(n, m_s, d)}{\partial m_s} + z(n, m_s, d) \frac{\partial z(n, -m_s, d)}{\partial m_s} \quad (C.5)$$

$$q_{s d} = \frac{4d}{N_+ N_-} \left\{ \frac{(n - 2d^2)(2n - 1 - 4d^2) - m_s^2}{\sqrt{n^2 - m_s^2 - 4nd^2 + 4d^4}} + \frac{(1 - n)n - 8d^4 + (8n - 6)d^2}{2d\sqrt{1 - n + d^2}} \right\} \quad (C.6)$$

For the calculation of the staggered susceptibility (see Appendix D) the second derivative of $q_s$ with respect to $m_s$ at $m_s = 0$ is required; the formula is:

$$q_{s m_s m_s} \equiv \left( \frac{\partial^2 q_s}{\partial m_s^2} \right)_{m_s = 0} = \frac{4n^2 - 8n + 8}{n^3(2 - n)^3} \left[ \sqrt{1 - n + d^2 + d} \right]^2 (n - 2d^2) - \frac{2(1 - n + 2d^2)}{n(2 - n)(n - 2d^2)}. \quad (C.7)$$

Appendix D: Staggered magnetic susceptibility for the paramagnet

In this appendix we derive a formula for the staggered magnetic susceptibility in the paramagnetic phase $\chi_s$:

$$\chi_s \equiv \left( \frac{\partial m_s}{\partial h_s} \right)_{h_s = 0}. \quad (D.1)$$
The procedure is as follows: the consistency equations (32)–(36) for the antiferromagnet in Section 2.2 allow for a paramagnetic solution in which $h_s = 0$ leads to $m_s = 0$ as well as $\tilde{\lambda}_s = 0$. Starting from this solution, we apply (at a fixed density) an infinitesimal staggered magnetic field $\delta h_s$. This introduces small changes in the other parameters, in particular $m_s$ and $\tilde{\lambda}_s$ acquire small values $\delta m_s$ and $\delta \tilde{\lambda}_s$ (the changes in $d$ and $\tilde{\mu}$ are irrelevant for the present discussion). Restricting ourselves to the $T = 0$ case, the two equations relating $\delta h_s$, $\delta m_s$ and $\delta \tilde{\lambda}_s$ are (expanding the consistency equations to first order in $\delta h_s$, $\delta m_s$ and $\delta \tilde{\lambda}_s$):

$$\delta m_s = \chi_{s,0} \delta \tilde{\lambda}_s,$$  \hspace{1cm} (D.2)

$$\delta \tilde{\lambda}_s = \delta h_s + b_s \delta m_s,$$  \hspace{1cm} (D.3)

where the following abbreviations are introduced:

$$\chi_{s,0} = \frac{2}{q} \int_{-\infty}^{-\tilde{\mu}/q} d\varepsilon \frac{N(\varepsilon)}{\varepsilon},$$ \hspace{1cm} (D.4)

$$b_s = 2q m_s \int_{-\infty}^{-\tilde{\mu}/q} d\varepsilon N(\varepsilon) \varepsilon.$$ \hspace{1cm} (D.5)

Here the parameter $q$ is $q_s$ taken at $m_s = 0$ (see Appendix C). Solving (D.2) and (D.3) for $\chi_s$ one has:

$$\chi_s = \frac{\delta m_s}{\delta h_s} = \frac{\chi_{s,0}}{1 - b_s \chi_{s,0}}.$$ \hspace{1cm} (D.6)

A similar result was obtained in Ref.\[10\].
References

[1] Hubbard J 1963 Proc. Roy. Soc. (London) A276 238, Gutzwiller M C 1963 Phys. Rev. Lett. 10 159, Kanamori J 1963 Progr. Theor. Phys. (Kyoto) 30 275, Anderson P W 1959 Phys. Rev. 115 2

[2] Dagotto E 1994 Rev. Mod. Phys. to be published

[3] Inui M and Littlewood P B 1991 Phys. Rev. B 44 4415

[4] Kotliar G and Ruckenstein A E 1986 Phys. Rev. Lett. 57 1362

[5] Metzner W and Vollhardt D 1989 Phys. Rev. Lett. 62 324

[6] Vollhardt D 1992 Strong-coupling approaches to correlated fermions in Proceedings Enrico Fermi Summer School, Varenna

[7] Oleś A M and Zaanen J 1989 Phys. Rev. B 39 9175

[8] Li T, Wölfle P and Hirschfeld P J 1989 Phys. Rev. B 40 6817

[9] Frésard R and Wölfle P 1992 Int. J. Mod. Phys. B 6 685, Erratum 6 3087

[10] Evans S M M 1992 Europhys. Lett. 20 53

[11] Denteneer P J H, Guozhong An and van Leeuwen J M J 1993 Phys. Rev. B 47 6256

[12] Denteneer P J H, Guozhong An and van Leeuwen J M J 1991 Europhys. Lett. 16 5

[13] Denteneer P J H 1994 Phys. Rev. B 49 6364

[14] Lavagna M 1990 Phys. Rev. B 41 142

[15] Fradkin E 1991 Field Theories of Condensed Matter Systems (Addison Wesley)

[16] Frésard R and Wölfle P 1992 J. Phys.: Condens. Matter 4 3625

[17] Vollhardt D 1984 Rev. Mod. Phys. 56 99

[18] Abramowitz M and Stegun I A 1970 Handbook of Mathematical Functions (New York: Dover)

[19] Möller B, Doll K and Wölfle P 1993 J. Phys.: Condens. Matter 5 4847

[20] Wolfram S 1991 MATHEMATICA, A system for doing mathematics by computer (Addison Wesley)

[21] Penn D R 1966 Phys. Rev. 142 350

[22] Hirsch J E 1985 Phys. Rev. B 31 4403
[23] Long M W 1991 in *The Hubbard Model: Recent Results*, M Rasetti ed. (World Scientific)

[24] von der Linden W and Edwards D M 1991 J. Phys.: Condens. Matter 3 4917

[25] ten Haaf D F B and van Leeuwen J M J 1992 Phys. Rev. B 46 6313

[26] Yedidia J S 1990 Phys. Rev. B 41 9397

[27] ten Haaf D F B, Brouwer P W, Denteneer P J H and van Leeuwen J M J 1994 unpublished.

[28] Belkhir L and Randeria M 1994 Phys. Rev. B 49 6829

[29] Hasegawa H 1990 Phys. Rev. B 41 9168

[30] Scalapino D J, White S R, and Zhang S C 1992 Phys. Rev. Lett. 68 2830
Scalapino D J, White S R, and Zhang S C 1993 Phys. Rev. B 47 7995

[31] Lilly L, Muramatsu A and Hanke W 1990 Phys. Rev. Lett. 65 1379, Mehlig B 1993 *ibid.* 70 2048, Lilly L, Muramatsu A and Hanke W 1993 *ibid.* 70 2049

[32] White S R, Scalapino D J, Sugar R L, Loh E Y, Gubernatis J E, and Scalettar R T 1989 Phys. Rev. B 40 506

[33] Moreo A, Scalapino D J, Sugar R L, White S R, and Bickers N E 1990 Phys. Rev. B 41 2313
| $4t/U$ | SBMF | HF  | HF/SBMF |
|-------|------|-----|---------|
| AF/WF/SF | 0.107 | 0.551 | 5.2 |
| AF/WF/PM | 0.183 | 0.548 | 3.0 |
| WF/SF/PM | 0.057 | 0.526 | 9.2 |

| $\delta$ |  |  |  |
|----------|---|---|---|
| AF/WF/SF | 0.067 | 0.25 | 3.7 |
| AF/WF/PM | 0.187 | 0.42 | 2.2 |
| WF/SF/PM | 0.275 | 0.45 | 1.6 |

| $\delta_c$ |  |  |  |
|----------|---|---|---|
| AF | 0.21 | 0.42 | 2.0 |
| F | 1/3 | 1 | 3.0 |

Table I. Comparison of location of tripod points (where three phases meet) in $(4t/U, \delta)$ phase diagram between Hartree-Fock approximation (HF) and slave-boson mean-field approximation (SBMF). Also the critical hole densities $\delta_c$ for antiferromagnetism (AF) and ferromagnetism (F) to occur in both approximations are compared. The last column gives the ratio of the HF and SBMF result in each case.
| $U/t$ | $\tilde{\lambda}$ | $m_s$ | $d$ | $-e_{AF}$ | $q_s(1, m_s, d)$ |
|---|---|---|---|---|---|
| 0 | 0 | 0 | 0.5 | 1.62114 | 1 |
| 1 | 0.042 | 0.093693 | 0.478519 | 1.38112 | 0.994185 |
| 2 | 0.24382 | 0.293750 | 0.444454 | 1.16716 | 0.980426 |
| 3 | 0.55345 | 0.461272 | 0.404445 | 0.986744 | 0.966375 |
| 4 | 0.94059 | 0.592152 | 0.364523 | 0.838877 | 0.956338 |
| 6 | 1.89519 | 0.768048 | 0.292458 | 0.623639 | 0.951682 |
| 8 | 2.98950 | 0.863161 | 0.235612 | 0.485104 | 0.959478 |
| 10 | 4.11613 | 0.913012 | 0.193926 | 0.393528 | 0.968953 |
| 12 | 5.23030 | 0.940510 | 0.163654 | 0.330002 | 0.976425 |
| 16 | 7.39950 | 0.967337 | 0.123965 | 0.248782 | 0.985641 |
| 20 | 9.51220 | 0.979394 | 0.099524 | 0.199420 | 0.990505 |
| 200.1 | 100 | 0.999800 | 0.009998 | 0.019976 | 0.999900 |

Table II. Self-consistent parameters for antiferromagnetic ground state at half-filling in slave-boson mean-field approximation as a function of $U/t$. The ground-state energy for $U/t = 0$ equals $-16/\pi^2$ exactly.
Table III. Spin-stiffness $\rho_s$ of the antiferromagnetic ground-state at half-filling as a function of $U/t$ as calculated in the Hartree-Fock approximation (HFA), the slave-boson mean-field approximation (SBMF), and from variational Monte Carlo calculations using the Gutzwiller wavefunction (GWVMC). For $U/t = 0$, $\rho_s$ equals $2/\pi^2$ exactly. For HFA and SBMF, results are for an infinitely large lattice, for GWVMC, results are for an $8 \times 8$ lattice, except for $U/t = 2, 3$ which are for $20 \times 20$ and $14 \times 14$ lattices, respectively (see also Ref.[11]).

| $U/t$ | $\rho_s^{\text{HFA}}$ | $\rho_s^{\text{SBMF}}$ | $\rho_s^{\text{GWVMC}}$ |
|-------|-----------------|-----------------|-----------------|
| 0     | 0.2026          | 0.2026          | —               |
| 1     | 0.2023          | 0.2012          | —               |
| 2     | 0.1960          | 0.1953          | 0.197           |
| 3     | 0.1820          | 0.1847          | 0.185           |
| 4     | 0.1650          | 0.1713          | 0.172           |
| 6     | 0.1332          | 0.1421          | 0.141           |
| 8     | 0.1090          | 0.1162          | 0.117           |
| 10    | 0.0912          | 0.0962          | 0.098           |
| 12    | 0.0781          | 0.0814          | 0.083           |
| 16    | 0.0602          | 0.0618          | —               |
| 20    | 0.0488          | 0.0497          | —               |
Figure captions

Figure 1 Ground-state \((4t/U, \delta)\) phase diagram of the Hubbard model on a square lattice, restricted to simple magnetic phases: paramagnet (PM), antiferromagnet (AF), weak (WF) and strong (SF) ferromagnet. \(\delta\) is the density of holes: \(1 - n\). (a) Construction diagram showing all continuous and first-order transition lines obtained in slave-boson mean-field approximation (SBMF), (b) phase diagram in SBMF, and (c) corresponding phase diagram in the Hartree-Fock approximation. Note the difference in scales of (b) and (c).

Figure 2 Helicity modulus \(\rho_s\) for the repulsive Hubbard model on a square lattice at half-filling as a function of \(U/t\). Shown are results from the Hartree-Fock approximation (HFA), from the slave-boson mean-field approximation (SBMF), and from variational Monte Carlo calculations using a Gutzwiller projected wave function (GWVMC, from Ref.[11]).

Figure 3 Effective hopping integral \(t_{\text{eff}}/t\) for the repulsive Hubbard model on a square lattice at half-filling as a function of \(U/t\). Shown are results from the Hartree-Fock approximation (HFA), the slave-boson mean-field approximation (SBMF), and Quantum Monte Carlo calculations (QMC, from Ref.[32]).

Figure 4 Effective hopping integral \(t_{\text{eff}}/t\) for the repulsive Hubbard model on a square lattice as a function of electron density \(n\). (a) For \(U/t = 4\), results are shown from the Hartree-Fock approximation (HFA), the slave-boson mean-field approximation (SBMF), and Quantum Monte Carlo calculations (QMC, from Ref.[33]), and (b) for \(U/t = 4, 8, 12,\) and 16 from SBMF calculations (QMC results for \(U/t = 4\) only). The dashed lines indicate the electron densities \(n_c\) for which in the phase diagram in Fig.1(a) a continuous PM/AF transition takes place. For \(U/t = 8, 12,\) and 16 the value of \(n_c\) is (approximately) equal to 0.8 in each case.