Symmetry breaking in the Hubbard model at weak coupling

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The phase diagram of the Hubbard model is studied at weak coupling in two and three spatial dimensions. It is shown that the Néel temperature and the order parameter in $d = 3$ are smaller than the Hartree-Fock predictions by a factor of $q = 0.2599$. For $d = 2$ we show that the self-consistent (sc) perturbation series bears no relevance to the behavior of the exact solution of the Hubbard model in the symmetry-broken phase. We also investigate an anisotropic model and show that the coupling between planes is essential for the validity of mean-field-type order parameters.

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The Hubbard model is one of the most important and most prominent theoretical models in modern condensed matter physics. Originally introduced in order to describe magnetism in transition metals, the Hubbard model has been most intensively investigated since Anderson’s proposal that the model should capture the essential physics of cuprate superconductors. The Hubbard-Hamiltonian

$$\mathcal{H} = -t \sum_{\langle ij \rangle \sigma} c_{i \sigma}^\dagger c_{j \sigma} + U \sum_i n_{i \uparrow} n_{i \downarrow}$$

(1)

describes itinerant electrons with spin $\sigma$ on a lattice with nearest neighbor sites $\langle ij \rangle$, interacting through short-ranged Coulomb repulsion $U$. The success of this relatively simple lattice model for mobile interacting electrons is based on its ability to explain a number of important phenomena in condensed matter physics. Among these are the (Mott-Hubbard) metal-insulator transition, antiferromagnetism, ferromagnetism, incommensurate phases, phase separation, and normal-state properties of high-$T_c$ materials.

In spite of the prominence of the Hubbard model in condensed matter theory and the deceptively simple two-parameter form of its Hamiltonian, comparatively little is known exactly (or even accurately) about its solution. In $d = 1$ the exact solution has been determined by the Bethe Ansatz technique. Even in the extreme weak coupling regime the ground state of the one-dimensional Hubbard model is nonperturbative, possessing a discontinuity at $U = 0^+$ where the Mott-Hubbard gap opens.

Much has recently been learned about the solution in high spatial dimensions ($d = \infty$), but even here the exact analytical solution is unknown, so that one has to recourse to perturbative or numerical methods. There is no doubt that the half-filled Hubbard model exhibits long-ranged antiferromagnetism in the high-dimensional limit, whereas the situation away from half-filling is less clear.

In $d = 2$ much is known from exact diagonalization or Monte Carlo simulation of finite systems. In addition much effort is spent on the analytical and numerical analysis of perturbative and nonperturbative results. While there seems to be now a consensus that at half-filling the ground state has long-range antiferromagnetic order, there are still controversies when the system is doped and – even at half-filling – concerning the question of whether there is or is not a precursor pseudogap.

In so far as numerical work on the three-dimensional Hubbard model has been carried out, the extrapolation of the results to the thermodynamic limit is clearly made difficult by the small linear system size. Much effort has been invested in the analysis of the phase diagram using perturbative techniques. In the strong coupling regime ($U \to \infty$), where the half-filled Hubbard model reduces to an effective Heisenberg model, high-temperature series expansions and $1/S$-expansions can reliably be used to estimate the Néel temperature and the ground state energy, respectively. However the analysis of the intermediate and weak coupling regime is much more difficult: For this regime a variety of approaches has been proposed, e.g., by Kakehashi, Logan, Cyrot, and Darré. These approaches all yield estimates for the Néel temperature which reduce to the Hartree-Fock result at weak coupling. However, it is well-known from studies of the Hubbard model, based on the $1/d$-expansion or the local approximation, that the Hartree-Fock approximation overestimates Néel temperature and order parameter in $d = 3$ by a factor of the order of four, even in the extreme weak-coupling limit. The precise value of this renormalization factor in $d = 3$ is as yet unknown.

The goal of this paper is, first, to present exact results for the broken-symmetry phase of the three-dimensional Hubbard model at weak coupling. In particular, we present asymptotically exact formulas for the Néel temperature and order parameter. It will be seen that this asymptotic formula also yields a useful approximation formula for the Néel temperature for all $U \lesssim D$, where $D = 12t$ is the band width of a three-dimensional hypercubic lattice. Second, we address sc perturbation theory for the broken-symmetry phase in low dimensions ($d = 2$) in the ground state. Our main result here is that sc perturbation theory breaks down altogether, and that low-order sc perturbation theory bears no relevance to the behavior of the exact solution of the Hubbard model in $d = 2$. We conclude that the antiferromagnetic order parameter cannot have a mean-field form. This result has
obvious relevance for theories of high-$T_c$ superconductivity, many of which are based on perturbation theory in strictly two-dimensional systems. Third, we investigate the order parameter of the anisotropic Hubbard model, where two-dimensional planes are weakly coupled in $c$-direction by a small hopping amplitude $t_\perp \ll t_\parallel$. We demonstrate that the sc perturbation series converges – however sluggishly – as long as the interplane hopping $t_\perp$ is finite.

Since the behavior of the Hubbard model even in the weak-coupling limit is nonperturbative one has to apply self-consistent theories. There are several ways of imposing self-consistency: The method at fixed order parameter $\Delta$ and some of its results are described in Ref. [33] for the special case of the Hubbard model in high spatial dimensions ($d \to \infty$). Here we extend these investigations to all finite dimensions. As described in Ref. [33], the order parameter $\Delta$ and the Néel temperature $T_N$ are determined by the roots of the optimization equation

$$\frac{df}{d\Delta} = 0,$$  

where $f$ is the free energy density. It then follows that one has to determine the order parameter from the self-consistency condition

$$\Delta = 2h_0 \int_0^\infty dt \, N_d(e) \tan \left[ \frac{1}{2} \eta(e) \right] \frac{\eta(e)}{\eta(e)},$$  

In Eq. (2) $h_0$ denotes the symmetry-breaking field, $\eta(e) = \text{sgn}(e) \sqrt{|e^2 + h_0^2|}$ the dispersion, and $\beta = 1/T$ the inverse temperature. $N_d(y)$ being the density of states in $d$ dimensions. It is important to note that in each order $h_0$ and $\Delta$ have to be determined self-consistently from the Hartree-Fock contribution and the fluctuations together to obtain systematic corrections to mean-field theory.

First we consider sc perturbation theory in the broken-symmetry phase in dimensions $d \geq 3$. Fortunately, although the evaluation of the various higher order diagrams in this approach at finite values of the interaction ($U > 0$) is difficult, if possible at all, the results at weak coupling (i.e., for $U \to 0$) are simple: For all $d \geq 3$ one finds that the exact value of the Néel temperature $T_N$ and the exact order parameter $\Delta$, can be expressed in terms of their Hartree-Fock equivalents and a scaling factor $q_d$. As is well-known, the Hartree Néel temperature is exponentially small for $U \to 0$: 

$$T_N^H \sim e^{I_d - 1/UN_d(0)},$$  

where $I_d$ can be expressed in terms of an integral,

$$I_d = \int_0^\infty dy \frac{1}{y} \left( \frac{\tanh y - 1 + N_d(y)}{N_d(0)} \right) - \ln 2.$$  

Now, we find that the exact expressions for $T_N$ and $\Delta(T)$ differ from the mean-field results by a scaling factor $q_d$:

$$T_N \sim q_d T_N^H (U \to 0),$$  

$$\Delta(T) \sim q_d \Delta^H (T/q_d) \quad (U \to 0).$$

For the special case $d = 3$ we now know from Ref. [33] that $q_\infty = \exp(-\gamma)$, where $\gamma = \sqrt{2}\arcoth(\sqrt{2})$, so that $q_\infty \approx 0.2875$. The renormalization factor $q_d$ for all $d \geq 3$ is determined by the second order diagrams only and can be conveniently written in the form of an exponential of a lattice sum:

$$q_d = e^{-S_d},$$  

where $S_d$ is given by

$$S_d = \frac{1}{t} \sum_{|j| \text{ even}} F_j^2 \int_0^\infty d\tau |G_j(\tau)|^2$$

and $F_j$ and $G_j(\tau)$ are integrals over Bessel functions:

$$F_j = \frac{1}{2\pi} \int_0^\infty dz \prod_{\ell = 1}^d [J_{|j_{\parallel}|}(z)]$$

$$G_j(\tau) = \frac{1}{\pi} \int_0^\infty dz \frac{\tau}{\tau^2 + z^2} \prod_{\ell = 1}^d [J_{|j_{\parallel}|}(z)].$$

This expression is formally exact for all $d > 2$. We have numerically evaluated the renormalization factor $q_d$ for $d = 3$ and find the following result:

$$q_3 = 0.2599.$$  

Thus, the exact Néel temperature and the exact order parameter are smaller than the Hartree-Fock predictions by almost a factor of four.

Several remarks are in order: (i) The term labeled by $j$ in the lattice sum $S_d$ stems from second order diagrams containing two Hubbard vertices a distance $|j|$ apart. (ii) Since we know from previous calculations in high dimensions [33] that sites at a relative distance $|j|$ give a contribution of order $d^{-|j|}$ to the free energy, one expects that the lattice sum $S_d$ converges extremely rapidly if $d$ is large. (iii) Keeping only the $j = 0$ term in $S_d$ corresponds to the local approximation of Ref. [33]. In $d = 3$ we find that $q_3^{(SC)} = 0.2673$. Comparison of $q_3^{(SC)} \approx 0.2673$ with the exact result $q_3 \approx 0.2599$ shows that the local approximation works very well even in $d = 3$. (iv) Note that odd lattice sites (i.e., interactions between the two sublattices) do not contribute to $q_d$ to leading order in $U$ for $U \to 0$. This is due to a different symmetry of the Green functions for odd and even values of $|j|$. (v) Also note that our result (3) for the renormalization factor diverge logarithmically for all even $|j|$.
The asymptotic result for the Néel temperature in Eq. (4) has a relevance beyond the pure weak coupling limit. This is particularly clear in infinite dimensions, where accurate quantum Monte Carlo data are available. A comparison of the Monte Carlo results with the appropriate asymptotic formula for \( d = \infty \) reveals excellent agreement for all \( U \lesssim D \). Therefore one expects that (4) yields an equally good approximation for \( U \lesssim D \) in \( d = 3 \). The phase diagram of the three-dimensional Hubbard model was calculated with a quantum Monte Carlo technique by Hirsch and Scalattar et al. A comparison of the Monte Carlo data from Ref. 24 with the expected behavior (4) reveals a significant discrepancy, suggesting (as was also pointed out in Refs. 24, 25) that the existing Monte Carlo estimates for \( T_N \) are too high. Improved Monte Carlo simulations show a significantly reduced Néel temperature. Yet it is still more than 15% higher than the asymptotic value (see Fig. 1). Our weak-coupling approximation formula (4) and the strong-coupling approximation formula \( T_{Nc} = 3.83 t^2 / U \) from Ref. 25 can hence serve as benchmarks for future Monte Carlo simulations.

Since the upper critical dimension of the Hubbard model is presumably \( d_\alpha = 4 \), one expects that the critical behavior of the order parameter in \( d = 3 \) is characterized by a nontrivial critical exponent for all \( U > 0 \). Yet the exact asymptotic behavior of \( \Delta(T) \) in (4) displays mean-field behavior near \( T_N \), with a critical exponent \( \beta = 1/2 \). These two observations can easily be reconciled by calculating the size \( \Delta T \) of the Ginzburg region in \( d = 3 \), which requires as input the correlation length \( \xi \) and the jump in the specific heat \( \Delta C \) at \( T_N \). An explicit calculation shows that \( \xi \) is exponentially large at weak coupling, \( \xi \propto [T_N(T_N - T)]^{-1/2} \), while \( \Delta C \) is exponentially small, \( \Delta C \propto T_N \). Combination gives for the relative size of the Ginzburg region: \( \Delta T / T_N \propto T_{Nc}^2 \), which is exceedingly small at weak-coupling and vanishes for \( U \to 0 \).

Now we address sc perturbation theory for the broken-symmetry phase in \( d = 2 \). Since \( T_N = 0 \) in \( d = 2 \), we focus on the renormalization of the ground state order parameter: \( \Delta = q_d \Delta^H \). Calculating only the second order contribution to Eq. (2) we find \( df_d / d\Delta \propto h_0 x^2 / 6 \) in the limit \( U \to 0 \) with \( x = \frac{U}{t} \ln \left( \frac{T}{h_0} \right)^2 \). The solution of the self-consistency equation (4) shows an interaction-dependent renormalization:

\[
\Delta = \frac{8t}{U} \left( 3 - \sqrt{3} \right) \exp \left( -\sqrt{\frac{4\pi^2 t(3 - \sqrt{3})}{U}} \right) .
\]  

In contrast to the result in \( d \geq 3 \), where \( q_d \) is constant, the renormalization factor in \( d = 2 \) vanishes exponentially as \( U \to 0 \). This result already indicates that the sc perturbation series in two dimensions has no small expansion parameter at weak coupling. Hence higher order fluctuation terms are important to decide whether the mean-field prediction for the form of the order parameter is at least qualitatively correct or does totally fail in \( d \leq 2 \) in the symmetry-broken phase.

To gain some insight into sc perturbation theory in higher orders we calculated bubble and ladder diagrams. We find

\[
\frac{df_{BL}}{d\Delta} \sim h_0 F_{BL}(x)
\]  

with the function

\[
F_{BL}(x) = 6 + x - x^2 - \frac{1}{2} \ln \left[ (1 + x)^{9(1 + \frac{1}{2})} (1 - x)^{(1 - \frac{1}{2})} \right]
\]  

for \( 0 < x < 1 \). The important result is that the optimization condition Eq. (2) has no roots for \( 0 < x < 1 \), apart from the high temperature solution \( \Delta = 0 \).

We comment on the results. (i) Our analysis shows that Hartree-Fock theory bears no relevance to the behavior of the Hubbard model in \( d = 2 \) at half-filling. The mean-field result is completely destroyed by quantum fluctuations. Hence the antiferromagnetic order parameter must have a completely different form: \( \ln(4t/h_0) \ll \sqrt{t/U} \). (ii) A calculation of bubble and ladder diagrams in \( d = \infty \) shows that all contributions \( f_n \) for \( n > 2 \) yield small corrections to \( q \) of the form \( q = q_\infty \exp \left[ 2N\infty(0)\gamma^2 U + O(U^2) \right] \), where \( \gamma \) has been defined above. (iii) Concerning the behavior of sc perturbation theory we conclude that only in dimensions \( d > 2 \) low-order sc perturbation theory is capable of describing the physics of the Hubbard model correctly. In low dimensions sc perturbation theory in the symmetry broken phase diverges. (iv) Remarkably, in \( d = 1 \) the structure of sc perturbation theory is exactly the same as in \( d = 2 \), now with \( x = \frac{U}{t} \ln \left( \frac{h_0}{T} \right) \) in Eq. (4).

The observation that sc second order perturbation theory gives even quantitatively exact results in \( d = 3 \) and diverges in \( d = 2 \) indicates that between two and
three spatial dimensions must be a transition where sc perturbation theory becomes inadequate. We introduced a weak hopping amplitude $t_\perp$ in c-direction. The anisotropy is then given by the dimensionless quantity $\lambda = t_\perp/t_\parallel \ll 1$ where $t_\parallel$ denotes the hopping in the planes. In this anisotropic three-dimensional model the renormalization factor can again be expressed as a lattice sum according to Eq. (3). However, the smaller $\lambda$ is the more sites have to be summed over. In the $j_1,j_2$-plane all points within a region $1/\lambda^2$ around the origin contribute with $\ln(1/\lambda)$ to the renormalization factor, yielding

$$q_\lambda = \exp \left( - \frac{\text{const.}}{\lambda^2 \ln(1/\lambda)} \right).$$

The renormalization factor is thus strongly reduced in less than three dimensions and zero in $d = 2$. This result demonstrates that the coupling to the third dimension is essential for mean-field theories to be qualitatively valid.

In summary, we have investigated the half-filled Hubbard model in two and three dimensions at weak coupling calculating systematic corrections to Hartree-Fock mean-field theory. We have shown that the mean-field antiferromagnetic Hartree-Fock solution does not yield exact results in the weak coupling regime. In particular, we showed that quantum fluctuation induced corrections make sc perturbation theory diverge in $d \leq 2$. In $d > 2$ the exact order parameter and Néel temperature differ from the mean-field result by a scaling factor.

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41. From a formal point of view the expansion parameter is $\lambda / t = U/\partial f/\partial h_\lambda$. This is small of order $U$ in $d > 2$ and of order unity below.