Phase diagram of the extended Hubbard model at weak coupling

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(Received 1 December 1995)

The Hubbard model including nearest neighbor interaction is studied at \( T = 0 \) on a \( d \)-dimensional hypercubic lattice \( (d \gg 1) \) close to half filling. For the model in \( d = \infty \) we derive the exact result that the ground state at weak coupling is phase separated. Results for lower dimensions are then derived in a 1/d expansion. To obtain these results we first consider possible second order transitions. One then finds that the broken-symmetry phase near half filling is incommensurate. However, the corresponding ground state has negative compressibility and is hence thermodynamically unstable. A Maxwell construction is used to construct the actual phase separated ground state, which consists of homogeneous lower-density and antiferromagnetic or charge density wave higher-density regions. It is shown that both the doping level below which phase separation occurs and the order parameter differ from the corresponding Hartree results by a renormalization factor \( q \). This renormalization factor \( q \) is calculated systematically up to \( O(1/d) \) in a 1/d expansion and turns out to be identical to the renormalization factor previously calculated for the low-temperature thermodynamics at half filling. [S0163-1829(96)06627-1]

I. INTRODUCTION

In recent years the Hubbard model has advanced to one of the most important standard models for interacting electrons on a lattice. Its Hamiltonian describes itinerant electrons, interacting through short-ranged (on-site) Coulomb repulsion. The success of the Hubbard model 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, incommensurate and, most recently, normal-state properties of high-\( T_c \) materials. Unfortunately, little is known exactly about the ground state or the thermodynamics of the Hubbard model. Nevertheless, the model at half filling is qualitatively well understood, mainly as a consequence of the exact solution in one dimension and several rather general rigorous results. The situation away from half filling is more severe. Here there exists basically only one rigorous result, due to Nagaoka, stating that the ground state for a single hole in a half-filled band is ferromagnetic in the extreme strong-coupling limit \( (U \to \infty) \). The purpose of the present paper is to extend the knowledge concerning the Hubbard model away from half filling. It presents exact results on the phase diagram of the slightly doped Hubbard model in the weak-coupling limit. These results will be derived for the Hubbard model on a hypercubical lattice in high dimensions \( (d \gg 1) \). The physical application kept in mind in deriving these results is that of the three-dimensional system. A short version of this paper was published previously as Ref. 12.

In this paper we will in fact consider a generalization of the pure Hubbard model, containing also nearest neighbor interaction. This more general model is usually referred to as the extended Hubbard model. Results for the pure Hubbard model are obviously contained in those for the extended model as special cases. The extended Hubbard model has at least two advantages over the pure model. (i) It has a richer phase diagram, containing, e.g., charge and spin density waves and various superconducting phases at half filling. (ii) It is definitely more realistic; this has been pointed out already by Hubbard, who argued for transition metals that the matrix element corresponding to nearest neighbor Coulomb repulsion is relatively large, so that its influence cannot a priori be neglected.

Accordingly, the extended Hubbard Hamiltonian has the form

\[
H = H_t + H_U + H_V + H_\mu,
\]

where

\[
H_t = -\frac{t}{\sqrt{2d}} \sum_{\langle ij \rangle, \sigma} (c_{i\sigma}^\dagger c_{j\sigma} \pm H.c.), \quad H_\mu = -\mu \sum_i n_i,
\]

\[
H_U = U \sum_i n_{i\uparrow} n_{i\downarrow}, \quad H_V = V \sum_{\langle ij \rangle} n_i n_j.
\]

Here \( c_{i\sigma}^\dagger \) (\( c_{i\sigma} \)) creates (destroys) an electron with spin \( \sigma \) at site \( i \), \( n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma} \), \( n_i = n_{i\uparrow} + n_{i\downarrow} \), and \( d \) is the space dimension. In the sum over bonds \( \langle ij \rangle \) in \( H_t \) and \( H_V \) it is understood that \( i \) and \( j \) are nearest neighbors and that every bond is counted only once. The grand canonical Hamiltonian (1) describes hopping of electrons (\( H_t \)), interacting with each other through on-site (\( H_U \)) and nearest neighbor (\( H_V \)) Coulomb repulsion. The prefactors in \( H_t \) and \( H_V \) are chosen such that a finite, nonvanishing energy contribution is obtained even in the limit \( d \to \infty \). Below we set \( t = 1 \) to fix the energy scale. Moreover, we consider only \( U > 0 \) and \( V > 0 \), since we assume Coulomb repulsion, but the results are valid in a wider range of parameters (see the discussion). The original Hubbard model corresponds to \( V = 0 \) in (1). Below we investigate the extended Hubbard model at weak coupling \( (U, V \downarrow 0) \), keeping the ratio

\[
v = V/U
\]
fixed. In order to obtain symmetry breaking, even in the limit $U, V \downarrow 0$, we focus on the nearly-half-filled band ($n = 1 - \delta$ with $\delta \ll 1$). As a result of particle-hole symmetry it suffices to consider only $\delta > 0$. It will become clear below that $\delta$ has to be exponentially small as a function of $U$ and $V$ in order to have symmetry breaking at weak interaction.

In this paper our aim is to obtain exact results for the extended Hubbard model in the weak-coupling limit $(U, V \downarrow 0)$. From previous work at half filling $^{17,18}$ we know that mean field theory (i.e., the Hartree-Fock approximation) does not become exact at weak coupling, not even in the limit of high dimensions ($d \to \infty$), where one would expect a mean field theory to be best. $^{19,20}$ Instead, to obtain exact results, one has to go to second order in perturbation theory. One then finds $^{17,18}$ that the exact results for the critical temperature and the order parameter at half filling differ from the Hartree predictions by a factor $q(v)$ of order unity. The renormalization factor $q(v)$ cannot in general be calculated exactly in finite dimensions (such as $d = 3$). However, it was shown in Refs. 17 and 18 that $q(v)$ can be calculated exactly in $d = \infty$; approximate results for finite-dimensional systems can then be obtained in a systematic $1/d$ expansion. In this paper we show that the same approach can be used to study the extended Hubbard model away from half filling.

The starting point of our investigations is therefore the infinite-dimensional limit. As far as I am aware, there are no exact (analytical) results for the Hubbard model in infinite dimensions away from half filling. However, there are several interesting results from Monte Carlo simulations of the less-than-half-filled Hubbard model in $d = \infty$, mainly due to Jarrell and co-workers. $^{21}$ From the Monte Carlo simulations it appears that incommensurate phases dominate the phase diagram away from half filling. However, it should be kept in mind that, in the simulations, the low-temperature and the weak- and strong-coupling regimes are inaccessible. In addition I would like to attract attention to the analytical work done by Uhrig and Vlaming $^{22}$ on interacting spinless fermions in $d = \infty$. The model of spinless fermions in $d = \infty$ is extremely simple in that the Hartree approximation becomes exact. Nevertheless, the phase diagram of this model turns out to be highly nontrivial. In fact we will see below that the weak-coupling behavior of spinless fermions in high dimensions is qualitatively very similar to that found in the Hubbard or extended Hubbard model.

The main results to be found below are the following. (i) The exact results for the order parameter and the critical doping concentration in the extended Hubbard model at weak coupling differ from the Hartree results by a renormalization factor of order unity. (ii) This renormalization factor turns out to be identical to that found for the model at half filling $^{17,18}$. Typically, the Hartree results are renormalized by a factor of $3 - 5$. The $1/d$ corrections in the renormalization factor are appreciable for realistic values of the ratio $v = V/|U|$. However, for the pure Hubbard model ($v = 0$) these corrections are relatively small. (iii) As for spinless fermions in $d = \infty$, $^{22}$ the ground state of the extended Hubbard model at weak coupling is phase separated. This is true also if $1/d$ corrections, for commensurate phases are taken into account. For the extended Hubbard model phase separation implies that regions with long-range antiferromagnetic (AFM) or charge density wave (CDW) order at density $n = 1$ coexist with disordered regions at the lower density $n = 1 - \delta < 1$. Here $\delta$ is the critical concentration of holes below which the phase separated state is stable. The conclusion of this work is therefore that the mechanism leading to symmetry breaking in the extended Hubbard model away from half filling corresponds to a first rather than a second order transition.

This paper is organized as follows. In the next section (Sec. II) we determine the phase diagram in the Hartree approximation. The influence of the fluctuations and the resulting renormalization of the Hartree results are then studied in Sec. III (perturbation theory) and Sec. IV (explicit results). In Sec. V we summarize and discuss the results. Technical details are deferred to the Appendixes.

II. THE HARTREE APPROXIMATION

This section consists of two parts. In the first part we discuss the Hartree approximation, restricting ourselves to purely antiferromagnetic or charge density wave phases. We calculate the critical doping concentration below which AFM or CDW order may occur, and also the order parameter and the ground state energy as a function of doping. In the second part, we investigate in general (but again within the Hartree approximation) the possible occurrence of incommensurate phases. The stability of the various phases and the resulting phase diagram are discussed. We consider ground state properties only. Technical details can be found in Appendix A (for AFM or CDW order) and in Appendixes B and C (for incommensurate phases).

A. Commensurate AFM and CDW phases

The Hartree approximation for a purely antiferromagnetic or CDW phase is defined by the decoupling scheme (A1) for the interaction terms in (1). The average density $\langle n_{\sigma} \rangle$ in (A1) contains the order parameter, which we denote by $\Delta$. The AFM phase is characterized by an alternating $z$ component of the spin. Hence $\langle n_{\uparrow} \rangle - \langle n_{\downarrow} \rangle = \Delta z$, where $\lambda = +1$ on one sublattice (labeled by $\{+\}$), and $\lambda = -1$ on the other (labeled by $\{-\}$). On the other hand, in the CDW phase the local density is modulated, $\langle n_{\uparrow} \rangle + \langle n_{\downarrow} \rangle = n + \lambda \Delta$. These requirements can be summarized as

$$\langle n_{\sigma} \rangle = \frac{1}{2} (n + \lambda r_\sigma \Delta),$$

where either $r_\sigma = 1$ (for a charge density wave), or $r_\sigma = \sigma$ (for antiferromagnetism). The order parameter $\Delta$ in the Hartree approximation can be calculated from the consistency requirement $\langle n_{\uparrow} \rangle = \frac{1}{2} (n \pm \Delta)$ if $\lambda \in \{\pm\}$. There are as usual two solutions: a trivial solution $\Delta = 0$ and a nontrivial solution $\Delta > 0$ that has a lower (Hartree) ground state energy if $\delta < \delta_1$, where $\delta_1$ is the Hartree prediction for the critical density of holes. We focus on the nontrivial solution below.

The Hartree approximation for the AFM and CDW phase at half filling was considered previously in Refs. 17 and 18. At half filling the temperature plays a similar role as is played in this paper by the concentration of holes. From the results of Refs. 17 and 18 we know that the Hartree order parameter $\Delta_0$ in the ground state at half filling is exponentially small, namely.
\[ \Delta_0 \sim \frac{\pi}{aU} \exp \left( I_d - \gamma - \frac{1}{2aUV_d(0)} \right) \quad (U,V \to 0). \]

This result is also important for the present paper, since (as we shall see below) \( \Delta_0 \) sets the scale for both the order parameter and the doping concentration away from half filling. The parameter \( \alpha \) in (3) is given by \( \alpha = 2\nu - \frac{1}{4} \) in the CDW and by \( \alpha = \frac{1}{4} \) in the antiferromagnetic phase, and \( \gamma = 0.577 \) is Euler's constant. In general dimensions \( d \geq 3 \) the constant \( I_d \) can be expressed in terms of an integral (see Ref. 18). For our purposes it suffices to quote the form of \( I_d \) in high dimensions, correct up to \( O(1/d) \) in the 1/d expansion,

\[ I_d = \frac{1}{2} \ln 2 + \frac{1}{2} \gamma - \ln \pi + \frac{1}{4d} + O(d^{-2}). \]

Its numerical value is \( I_d = 0.1836 + 1/4d \).

The order parameter \( \Delta(\delta) \) away from half filling (i.e., for \( \delta > 0 \)) is calculated in Appendix A. One finds that \( \Delta(\delta) \), too, is exponentially small as a function of \( U \) and \( V \). More explicitly,

\[ \Delta(\delta) = \Delta_0 \sqrt{1 - \delta \delta_1}, \quad \delta_1 = \nu_d(0)H_0. \]

Here \( H_0 = aU\Delta_0 \) is the Hartree gap parameter at half filling. The critical concentration \( \delta_1 = \nu_d(0)H_0 \) in (5) has been identified from the criterion \( \Delta(\delta_1) = 0 \). The same value \( \delta_1 \) for the critical density could have been obtained from the homogeneous phase, by calculating the divergence of the random-phase approximation (RPA) susceptibility at wave vector \( q = Q = (\pi, \pi, \pi, \ldots) \). Note that the order parameter as a function of doping has a very simple form, with a mean field critical exponent of 1/2 near \( \delta = \delta_1 \). Also note that \( \Delta(\delta) \) has a nonvanishing slope at \( \delta = 0 \).

Similarly one can calculate the energy gain per site \( E_S \) due to symmetry breaking (for details, see Appendix A),

\[ E_S(\delta) = -\frac{1}{2}(aU\Delta_0)^2\nu_d(0) \left( 1 - \frac{\delta}{\delta_1} \right)^2. \]

This result shows that symmetry breaking indeed leads to an energy gain and that this energy gain is exceedingly small, of order \( U^2\Delta_0^2 \). Equation (6) also shows that the lowest ground state energy is obtained for the phase with the largest value of \( \alpha \). This shows that, as at half filling, the system is in the CDW phase for \( \nu > \frac{1}{4} \) and in the SDW phase for \( \nu < \frac{1}{4} \), at least in the Hartree approximation.

Thermodynamically, the difference between the ground state energy \( E(\delta) \) at concentration \( \delta \) and the ground state energy \( E(0) \) at half filling is even more interesting. The reason is that this quantity reveals the density dependence of the energy (which is important, see below). The energy difference \( E(\delta) - E(0) \) is calculated in Appendix A. The result is

\[ E(\delta) - E(0) = -(2V + \frac{1}{2}U)\delta + 2\nu_d(0)H_0^2\Phi(\delta/\delta_1), \]

where \( H_0 \) is defined below (5) and

\[ \Phi(x) = \frac{1}{2}x(1 - \frac{1}{2}x) \quad (x < 1) \]
\[ = \frac{1}{4}(1 + \frac{1}{2}x^2) \quad (x > 1). \]

FIG. 1. The energy of the various phases as a function of doping. At small doping (\( 0 < \delta \delta_1 < 1 \)) the paramagnetic phase (short dashed curve) has the highest energy. The energy can be lowered by antiferromagnetic symmetry breaking (long dashed curve) or incommensurate symmetry breaking (dashed curve), but these phases are unstable: the energy is nonconvex as a function of density. A Maxwell construction (the straight solid line, whose produced part is long-short-short dashed) then yields a thermodynamically stable state for \( 0 < \delta \delta_1 < \sqrt{2} \). This stable state is phase separated. Thus the actual ground state energy is for all \( \delta \delta_1 > 0 \) given by the solid curve.

A sketch of \( E(\delta) \), or rather \( \Phi(\delta/\delta_1) \), is given in Fig. 1. The first term on the right in (7) is due to the chemical potential. The second term is physically much more interesting and reveals that the ground state energy is not convex as a function of particle number, at least not for \( \delta < \delta_1 \). Since this is thermodynamically impossible (it implies a negative compressibility) one concludes immediately that pure AFM or CDW symmetry breaking is not stable.

\textit{A priori} there are two possible solutions to this problem. Either the assumption, made implicitly above, that the phase transition is second order is correct but the broken-symmetry phase has more complicated (incommensurate) order, or alternatively the transition is not second order. We address the latter possibility first. The results from the AFM/CDW phase can be used to construct a thermodynamically stable state with the use of the Maxwell construction (see the straight line in Fig. 1). Physically the Maxwell construction implies that the actual (stable) state consists of a mixture of antiferromagnetically ordered or CDW regions (at density \( n = 1 \)) and disordered regions (at density \( n = 1 - \delta_3 \)). The critical density of holes \( \delta_3 \), below which such a phase separated state would be stable, follows from (7) as \( \delta_3 = \sqrt{2} \delta_1 \). The question to be investigated below is whether some incommensurate phase might possibly be stable at still higher values of \( \delta \).

\section*{B. Incommensurate phases in \( d = \infty \)}

In the following we consider general incommensurate phases, where the order parameter in the broken-symmetry phase is characterized by the wave vector \( q \neq Q \). The sim-
plest way to investigate possible incommensurate symmetry breaking is to calculate the spin-dependent density-density susceptibility in the RPA approximation in the homogeneous phase. The calculations are elementary and very similar to those carried out for spinless fermions by Uhrig and Vlaming.\textsuperscript{22} One finds that the homogeneous phase becomes unstable at wave vector $q$ if one of the following two conditions is met:

\begin{align}
1 &= U\chi_0(q), \quad (8a) \\
1 &= [-4V\rho_q - U]\chi_0(q), \quad (8b)
\end{align}

where $\chi_0(q)$ is identical to the density-density correlation function for the noninteracting system and the parameter $\rho_q$ is defined as

$$
\rho_q \equiv \frac{1}{d} \sum_{n=1}^{d} \cos(q_n) = -\frac{1}{\sqrt{2d}} e^q . \quad (9)
$$

The RPA criterion can be analyzed for small interaction, as was done for spinless fermions in Ref. 22. The analysis is simple only strictly in $d = \infty$, since then the non-interacting susceptibility $\chi_0(q)$ depends upon the incommensurate vector $q$ only through the one-dimensional parameter $\rho_q$. One can calculate the optimal value $\rho_{\text{opt}}$ of $\rho_q$, i.e., the value for which the susceptibility $\chi_0(q)$ diverges first. As a result one finds a relation between $\rho_{\text{opt}}$ and the “effective” chemical potential $\mu_0 \equiv \mu - (2V + 2U)n$,

$$
\mu_0 / \sqrt{1 + \rho_{\text{opt}}} = s_2 , \quad (10)
$$

where $s_2$ is implicitly given by $2s_2 F(s_2) = 1$, with $F(x) = e^{-x^2} \int_0^\infty dt e^{xt^2}$. Its numerical value is $s_2 \approx 0.924$. Precisely the same relation (10) was found in Ref. 22 for spinless fermions. Note that at small $U$ (where $\delta$ and $\mu_0$ are exponentially small) $\rho_{\text{opt}}$ is close to $-1$, so that $q$ is close to $Q$. Therefore the RPA criterion basically simplifies to $1 = 2a U\chi_0(q)$, with $\alpha = \frac{1}{2}$ or $\alpha = 2 \delta - \frac{1}{2}$ for incommensurate spin or charge density waves, respectively.

The extra relation between $\mu_0$ and $\rho_{\text{opt}}$ can now be used to determine the critical concentration of holes $\delta_2$ for the dominant incommensurate phase. The result is

$$
\delta_2 / \delta_1 = s_2 e^{\Gamma + \gamma/2} ,
$$

where $\gamma = 0.5772$ is Euler’s constant and $\Gamma$ is given by

$$
\Gamma = \frac{1}{2} \int_0^1 \frac{dt}{t} \left( \frac{e^{-s_2^2 t}}{\sqrt{1-t}} - 1 \right) = 0.0356 .
$$

Numerically this implies $\delta_2 / \delta_1 \approx 1.278$, so that (if only second-order transitions could occur) the broken-symmetry phase would have incommensurate order with $\rho_q$ satisfying (10) at $\delta = \delta_2$. However, from the analysis above we know that phase separation (a first order transition) can occur already at a concentration of holes $\delta_3$, satisfying $\delta_3 / \delta_1 = \sqrt{2}$. The conclusion is therefore that at weak coupling $\delta_1 < \delta_2 < \delta_3$, so that incommensurate phases are suppressed and phase separation dominates: $\delta_2 = \max\{\delta_1, \delta_3, \delta_2\} = \delta_3$. We note that, at the Hartree level, the critical densities $\delta_1$, $\delta_2$, and $\delta_3$, found for the extended Hubbard model, are precisely twice the corresponding critical densities for spinless fermions.

Although these arguments clearly demonstrate that a transition into a phase separated state must occur, strictly speaking phase separation need not occur precisely in the manner sketched above, as a coexistence of AFM/CDW and homogeneous domains. One could imagine more complicated scenarios, such as coexistence of incommensurate and homogeneous domains (at larger doping), purely incommensurate phases (at intermediate doping) and coexistence of incommensurate and AFM/CDW domains (at low doping). Such scenarios depend crucially on the form of the energy as a function of doping in the incommensurate broken-symmetry phase.

To rule out such more complicated scenarios we investigate $E(\delta)$ in the broken-symmetry phase (i.e., for $\delta < \delta_2$). We consider the case of an incommensurate spin density wave\textsuperscript{23} at wave vector $q \neq Q$. With the usual definition of the Heisenberg spin, $S_i = \frac{1}{2} \sum_{\alpha \beta} \sigma_{\alpha i} \sigma_{\beta i}$ (where $\sigma$ represents the Pauli matrices), the order parameter takes the form

$$
\langle S_i^x \rangle + i \langle S_i^y \rangle = \frac{1}{2} \Delta e^{i q \cdot r} . \quad (11)
$$

For $q = \mathbf{Q}$ this reduces to the commensurate (antiferromagnetic) order parameter, discussed above. The diagonalization of the Hartree Hamiltonian for the incommensurate SDW phase and the derivation of equations for the order parameter, the chemical potential, the energy, and the Green functions are discussed in Appendix B. For general values of the interaction, these equations are still complicated, even in $d = \infty$. Fortunately, a further simplification occurs in the weak-coupling limit, where these equations take a form involving only relatively simple one-dimensional integrals, which form an excellent starting point for both analytical calculations and numerical work. The derivation of these simpler expressions is deferred to appendix C. Here we present the main results.

We start with a discussion of analytical results valid in the critical region ($\Delta \to 0$, or $\delta \to \delta_2$). For $\Delta \to 0$, the result for $\delta_2$, obtained from the calculation in the broken-symmetry phase, obviously ought to agree with the critical point obtained from the divergence of the susceptibility in the homogeneous phase. That this is indeed the case follows immediately from Eq. (B6). One finds that, for $\Delta \to 0$, the equation for the order parameter reduces to the form $1 = U \chi_0(q)$, where $\chi_0(q)$ is the density-density correlation function for the noninteracting system. Therefore the $\delta_2$ criterion derived from the broken-symmetry phase agrees with the RPA criterion (8a), as it should. More detailed information about the critical region can be obtained from Eqs. (C4)–(C6). For this purpose we introduce a reduced doping fraction, gap parameter, chemical potential, and incommensurability as follows:

$$
D = \delta / \delta_2 , \quad P = h_0 / \delta_2 , \quad M = |\mu_0| / \delta_2 , \quad R_{\text{opt}} = (1 + \rho_{\text{opt}}) / 2 \delta_2^2 . \quad (12)
$$

Here $h_0 = \frac{1}{2} U \Delta$ is the Hartree gap parameter away from half filling ($n \neq 1$). The advantage of the reduced order parameter $P$, chemical potential $M$, and incommensurability $R_{\text{opt}}$ is
that these quantities remain finite in the limit $U \rightarrow 0$. One finds from (C4)–(C6) the following asymptotic results for $\delta \rightarrow \delta_2$, or $D \uparrow 1$:

$$P \sim -\sqrt{\pi(1-D)},$$

$$M \sim \sqrt{\pi/2} + O((1-D)^{3/2}) \quad (D \uparrow 1),$$

$$R_{\text{opt}} \sim \frac{\pi}{4} [(s_2)^{-2} + D - 1].$$

The constant $s_2$ has been introduced below (10). It is seen that $P$, $M$, and $R$ smoothly approach their respective critical values as $D \uparrow 1$.

Next we discuss the low doping limit ($\delta \sim \delta_2 \rightarrow 0$). The three coupled equations, derived in Appendix C, can be solved analytically also in this limit. One finds that the optimal solution has the properties $\Delta \rightarrow \Delta_0$, $\mu_0 \rightarrow -H_0$, and $\rho_{\text{opt}} \rightarrow -1$, or $q \rightarrow Q$. More precisely, in terms of the reduced variables $D$, $P$, $M$, and $R_{\text{opt}}$:

$$P \sim P_0 - \sqrt{\pi/2} D,$$

$$M \sim P_0 - \sqrt{\pi/2} D \ln(1/D) \quad (D \rightarrow 0),$$

$$R_{\text{opt}} \sim \frac{\pi}{2} D^2 \ln(1/D),$$

where $P_0$ is the value of $P$ at half filling: $P_0 = \alpha U \Delta_0 / \delta_2$. Its numerical value is $P_0 \approx 1.96125$. From (14) it is clear that the approach to the AFM state is continuous as a function of density. In particular, the first derivative of the energy with respect to hole density follows from (14) as

$$\frac{\partial E}{\partial \delta} (\delta \rightarrow 0) = -\mu (\delta \rightarrow 0) = -(2V + \frac{U}{2}) + H_0. \quad (15)$$

This is identical for small $\delta$ to (7), so that the ground state energy of the optimal incommensurate phase is also necessarily nonconvex as a function of particle number. In fact (14) implies $\partial^2 E/\partial \delta^2 \sim -\sqrt{\pi/2} \ln(1/\delta) \rightarrow -\infty$ so that the compressibility of this phase is negative (and divergent) at small doping.

To check whether the compressibility of the incommensurate phase is negative in the entire interval $0 < D < 1$ I also solved the coupled equations of appendix C numerically. The results are presented in Fig. 2. Figure 2 gives the order parameter, the chemical potential, and the optimal incommensurability. The results have been normalized such that their maximum values are unity. The maximum is obtained for $D = 0$ (in the case of the order parameter and the chemical potential) or $D = 1$ (in the case of the incommensurability). The energy as a function of doping, or rather the function $\Phi(x)$ in (7), has also been calculated. The result has been added to Fig. 1 as the dashed line. The numerical solution is seen to interpolate smoothly between the asymptotic results obtained analytically in the low-doping region and the critical region. Moreover, the compressibility is indeed found to be negative on the entire interval $0 < D < 1$.

Clearly the negative sign of the compressibility for all $\delta < \delta_2$ implies that the incommensurate phase, too, cannot be stable. Consequently, the more complicated scenarios, discussed above, can be ruled out: The stable (phase separated) ground state, as obtained from the Maxwell construction, is indeed a mixture of purely antiferromagnetic and homogeneous domains. Thus the actual critical density of holes $\delta_c$ below which symmetry breaking is stable is at weak coupling determined by phase separation, so that $\delta_c = \delta_2$.

The main question to be investigated below is whether the phase diagram found above in Hartree approximation survives if one takes fluctuations into account.

### III. SECOND ORDER PERTURBATION THEORY

In the following two sections we address the effects of fluctuations on the Hartree (or, for incommensurate phases, Hartree-Fock) results, discussed in the previous section. The influence of fluctuations can be studied in self-consistent second order perturbation theory. There are various equivalent ways to do this.\textsuperscript{24–26} Here we use the so-called perturbation theory at constant order parameter\textsuperscript{24} that was applied to the half-filled extended Hubbard model in Refs. 17 and 18. We restrict the discussion to the AFM and CDW phases, which are simplest. Results for incommensurate phases will simply be summarized at the end. To distinguish exact weak-coupling results from results obtained in the Hartree approximation, we will henceforth label all Hartree results by a superscript $H$. We discuss the perturbation theory in the AFM/
CDW phase first. Subsequently we comment on modifications occurring for incommensurate phases.

A. Commensurate AFM or CDW phases

Perturbation theory at constant order parameter is based on an expansion of the free energy per site \( f(U,V,\Delta) \) in powers of \( U \) and \( V \) at a fixed value of the order parameter \( \Delta \) and a fixed concentration of holes \( \delta \):

\[
f(U,V,\Delta,\delta) = f_0 + f_1 + f_2 + \cdots. \tag{16}
\]

Since we consider only ground state properties, the free energy coincides with the ground state energy. The functions \( f_n(\Delta,\delta) \) in (16) depend implicitly on \( v \) and \( T \). The order parameter in (16) is kept fixed by introducing a Lagrange parameter \( h(U) \), which couples linearly to the staggered magnetization (in the SDW case) or to the staggered charge density (in the CDW case). Similarly, the chemical potential \( \mu(U) \) is tuned such that the number of particles remains fixed. At small \( U \) the Lagrange multipliers \( h(U) \) and \( \mu(U) \) have expansions of the form \( h(U) = h_0(\Delta,\delta) + h_1(\Delta,\delta)U + \cdots \) and \( \mu(U) = \mu_0(\Delta,\delta) + \mu_1(\Delta,\delta)U + \cdots \), respectively.

For the AFM and CDW phases the contributions \( f_n \) to the free energy per site are for \( n = 0,1,2 \) given by

\[
f_0 = h_0 \Delta - 2 \int_{\epsilon_m}^\infty d\epsilon \nu_\epsilon(\epsilon) \eta_\epsilon, \tag{17a}
\]

\[
f_1 = \left( \frac{1}{2} U + V \right) n^2 - \frac{1}{2} a U \Delta^2 - 2 V \left[ G_1(0) \right]^2, \tag{17b}
\]

\[
f_2 = -\frac{1}{2} \frac{1}{\beta N} \lim_{\beta \to \infty} \int_{\epsilon_m}^\beta \int_{\epsilon_m}^\beta d\tau_1 d\tau_2 \langle [\overline{H}_U(\tau_1) + \overline{H}_V(\tau_1)]
\]

\[
\times [\overline{H}_U(\tau_2) + \overline{H}_V(\tau_2)] \rangle_0. \tag{17c}
\]

Here \( \eta_\epsilon \) and \( \epsilon_m \) are defined by \( \eta_\epsilon = \text{sgn}(\epsilon) \sqrt{\epsilon^2 + h_0^2} \) and \( \epsilon_m = \sqrt{\mu_0^2 - h_0^2} \), respectively, and \( G_1(0) \) in \( f_1 \) is the Hartree Green function \( G_{1i}(\tau) \) for nearest neighbors \( i \) and \( j \) and \( \tau = 0 \). The operators \( \overline{H}_U \) and \( \overline{H}_V \) in \( f_2 \) represent the fluctuations in \( H_U \) and \( H_V \) (i.e., the Hartree and the Fock terms have been subtracted). The average \( \langle \cdots \rangle_0 \) refers to connected diagrams, which are to be calculated using Hartree Green functions with chemical potential \( \mu_0 = \mu(0) \) and gap parameter \( h_0 = h(0) \). Here \( \mu_0 \) and \( h_0 \) depend in turn on the density \( n = 1 - \delta \) and the order parameter \( \Delta \) through the consistency relations

\[
\delta = 2 \int_{\epsilon_m}^{\epsilon_m} d\epsilon \nu_\epsilon(\epsilon), \tag{18a}
\]

\[
\Delta = 2 h_0 \int_{\epsilon_m}^{\epsilon_m} d\epsilon \nu_\epsilon(\epsilon)/\eta_\epsilon. \tag{18b}
\]

Note that the parameter combination \( \epsilon_m \) is completely determined by the density \( \delta \) and, hence, that \( \Delta \) can be varied by tuning \( h_0 \) while keeping \( \epsilon_m \) fixed.

The calculation of the second order contribution \( f_2 \) up to first order in \( 1/d \) requires the calculation of several diagrams. These diagrams are the same as those that had to be calculated for the half-filled band; see Fig. 1 of Ref. 17. The only first order diagram [diagram (a) of Ref. 17, Fig. 1], represents the Fock term. Diagrams (b)—(e) correspond to the various second order diagrams. In Ref. 17 it was shown that contributions from the third order diagrams, represented by (f) in Fig. 1, can be shown to be vanishingly small for \( U \to 0 \). As in Ref. 17 it suffices to know the Green functions for short distances only \( (|s| = 0,1) \), if one wants to calculate diagrams up to order \( 1/d \).

When the various diagrams have been calculated and the ground state energy \( f \) is known, the equilibrium value of \( \Delta \) is determined by minimization of the ground state energy at fixed \( (U,V,\delta) \):

\[
0 = \frac{df}{d\Delta} = \frac{df}{dh_0} \frac{dh_0}{d\Delta} + \frac{df}{d\Delta}. \tag{19}
\]

The restriction that the density is to remain fixed in calculating the derivatives implies on account of (18a) that \( \epsilon_m \) remains fixed. Below we will denote the ground state energy per site for the equilibrium value of \( \Delta(\delta) \) by \( E(\delta) \), i.e.,

\[
E(\delta) = f(U,V,\Delta(\delta),\delta). \]

Once \( \Delta(\delta) \) has been determined from (19), the result can be used to calculate the actual critical concentration of holes \( \delta_1 \) and the actual phase diagram of the slightly doped extended Hubbard model at weak coupling. The results for \( \delta_1 \) and for the phase diagram will be presented in the next section.

B. Incommensurate phases

We end this section with a remark on perturbation theory in the incommensurate SDW phase in \( d = \infty \). The calculations in this case are formally very similar to those sketched above, but the equations are more difficult in detail. For instance, in (17) the zeroth order term \( f_0 \) in the incommensurate case contains a double energy integral instead of the simple \( \epsilon \) integral in (17a). The Fock term in \( f_1 \) can be dropped, since we consider only \( d = \infty \). Similarly in \( f_2 \), the nearest neighbor interaction \( \overline{H}_V \) can be dropped and only \( \overline{H}_U \) remains. The second order term involving \( \overline{H}_V \), however, now leads to \textit{four} diagrams, since the Green functions are nondiagonal in spin space. The consistency relations (18), too, are more complicated and take the form of twofold energy integrals.

IV. CALCULATION OF THE SECOND ORDER CORRECTIONS

The diagrams (a)–(e), describing the second order contribution to the ground state energy, have to be calculated with the use of the Hartree Green functions, given in Appendix A. Fortunately, the present calculations (for the ground state away from half filling) are very similar\(^{17,18}\) to those previously\(^{17,18}\) carried out for the half-filled case at \( T = 0 \). For details we refer to Refs. 17 and 18. Here we simply summarize the results.
A. Commensurate AFM or CDW phases

As in Refs. 17 and 18 we introduce the contribution \( f_v \) to the total ground state energy \( f \), due to diagram \( \nu \) (see Fig. 1 of Ref. 17; \( \nu = a, \ldots, e \)). Furthermore, we introduce the derivative of \( f_v \) with respect to the field \( h_0 \),

\[
B_v(h_0, \delta) = \frac{1}{h_0} \left( \frac{\partial f_v}{\partial h_0} \right) \delta.
\]  
(20)

The main reason for introducing \( B_v(h_0, \delta) \) is that one needs the derivative to determine the equilibrium value of \( \Delta \); see (19).

It now turns out that in the limit \( U \downarrow 0 \) the numerical values of the diagrams (a)–(e) in Fig. 1 of Ref. 17 are simply identical to the corresponding values at half filling.\(^{15}\) This simplification obviously occurs only in the limit \( U \downarrow 0 \); for any \( U > 0 \) results will in general be different. The reason why (for \( U \downarrow 0 \)) the \( T = 0 \) diagrams away from half filling lead to the same numerical contributions as the \( T \geq 0 \) diagrams for \( n = 1 \) is that the energy cutoffs \( \mu_0 \) (for \( n < 1 \)) and \( T_c \) (for \( n = 1 \)) have the same exponential \( U \) dependence for small \( U \). For our purposes it therefore suffices to summarize the results of Refs. 17 and 18:

\[
B_d(h_0, \delta) = -\frac{u}{2\pi \alpha d},
\]  
(21a)

\[
B_s(h_0, \delta) \sim \gamma_d / \alpha^2,
\]  
(21b)

\[
B_c(h_0, \delta) = O(U/d),
\]  
(21c)

\[
B_d(h_0, \delta) = \frac{4v^2 \gamma_s}{\alpha^2 d},
\]  
(21d)

\[
B_s(h_0, \delta) \sim \frac{u}{\alpha d} \left( \gamma_s - \frac{1}{\sqrt{2\pi}} \right),
\]  
(21e)

These results are valid only at weak coupling, i.e., in the limit \( U \downarrow 0 \). We note that the Fock diagram (a) is small (of order \( 1/d \)), that diagram (b) is the only second order diagram in Fig. 1 of Ref. 17 that survives in \( d = \infty \), and that diagram (c) is negligibly small compared to the other diagrams for small \( U \). The constant \( \gamma_d \) appearing in (21) is given by\(^{17,18}\)

\[
\gamma_d = \gamma_s - \frac{3}{32d} \left( \gamma_s + \frac{1}{3\sqrt{2\pi}} \right) + O(d^{-2}),
\]  
(22)

where \( \gamma_s = (1/2\sqrt{\pi})\ln(\sqrt{2} + 1) \).

It immediately follows from (21) that \( \overline{B} = \Sigma_v B_v \), which represents the derivative with respect to \( h_0 \) of the energy correction \( f = \Sigma_v f_v \), is given by

\[
\overline{B}(h_0, \delta) = \frac{1}{h_0} \frac{\partial f}{\partial h_0} \sim \overline{C}(U \rightarrow 0),
\]  
(23)

where the constant \( \overline{C} \) is defined as

\[
\overline{C} = \frac{v}{\sqrt{2\pi \alpha d}} + \frac{\gamma_d}{\alpha^2} + \frac{4v^2 \gamma_s}{\alpha^2 d} + \frac{v}{\alpha^2 d} \left( \gamma_s - \frac{1}{\sqrt{2\pi}} \right).
\]  
(24)

The total ground state energy is the sum of the Hartree contribution and the diagrammatic corrections: \( f = f_H^{\infty} + \overline{f} \), where \( \overline{f} \) can be written as

\[
\overline{f}(h_0, \delta) = \overline{f}(0, \delta) + \frac{1}{2} \overline{C} h_0^2.
\]  
(25)

The minimization condition (19) now yields an equation for the Lagrange multiplier \( h_0 \) as a function of the order parameter \( \Delta \):

\[
h_0 \sim \alpha U \Delta/(1 + \overline{C} dh_0/d\Delta).
\]

From (18b) we know for small \( U \) that \( dh_0/d\Delta \sim \alpha U \), so that, just as in Refs. 17 and 18,

\[
h_0 = \alpha^* U \Delta,
\]  
(26a)

\[
\alpha^* \sim \alpha - \alpha^* U \overline{C} + \cdots.
\]  
(26b)

Insertion of (26a) into (18b), and comparison with Eq. (A10) for the order parameter in the Hartree approximation shows that \( \Delta(\delta) \) has the same form as \( \Delta^{\infty}(\delta) \) if in addition one replaces \( \alpha \rightarrow \alpha^* \).

As a consequence of (A10) one finds that the exact critical concentration of holes, the exact order parameter \( \Delta \), and the exact energy gain due to symmetry breaking can be expressed in terms of their Hartree equivalents and a scaling factor

\[
q(\nu) = e^{-\overline{C}/2\nu_0(0)} = e^{-C_0 - C_1^{(n=1)} d^{-1}},
\]  
(27)

with

\[
C_0 = \frac{1}{2\sqrt{2\alpha^2}} \ln(\sqrt{2} + 1),
\]  
(28)

\[
C_1 = \left( \frac{\alpha - 1}{64\alpha^2} - 1 \right) + C_0 \left( \frac{1}{32} + v + 4v^2 \right).
\]  
(29c)

The scaling factor \( q \) is identical to that occurring for the half-filled case in Refs. 17 and 18. The exact expressions for \( \delta_1, \Delta(\delta), \) and \( E_S(\delta) \) are now given by

\[
\delta_1 \sim q \delta_1^{H},
\]  
(29a)

\[
\Delta(\delta) \sim q \Delta^{H}(\delta | q) (U, V \downarrow 0),
\]  
(29b)

\[
E_S(\delta) \sim q^2 E_S^{H}(\delta | q).
\]  
(29c)

Clearly the system can still gain energy by breaking the symmetry \( (E_S < 0) \), but all physical properties (the critical doping concentration, the order parameter, the energy gain \( E_S \), etc.) are strongly affected by quantum fluctuations.

The \( \delta \) dependence of the ground state energy is particularly clearly revealed if one considers the energy difference \( E(\delta) - E(\delta = 0) \) between the system at density \( \delta \) and that at half filling \( (\delta = 0) \). We note that the ground state energy \( E(\delta) \) of the system at density \( \delta \) can be written as

\[
E(\delta) = f(\Delta(\delta), \delta)
\]

\[
= f(0,0) + [f(0, \delta) - f(0, 0)] + [f(\Delta(\delta), \delta) - f(0, \delta)]
\]

\[
= f(0,0) + E_D(\delta) + E_S(\delta).
\]  
(29d)
From this result it is not difficult to show that the energy difference \( E(\delta) - E(0) \) is given by

\[
E(\delta) - E(0) = E_D(\delta) + E_S(\delta) - E_0(0)
\]

\[
= - (2V + \frac{1}{2}U) \delta + 2 \nu_0(0) H_0^2 \Phi(\delta/\delta_1),
\]

(30)

where \( \Phi(x) \) is given below Eq. (7) for \( \delta < \delta_1 \) and \( \delta > \delta_1 \), respectively. In the derivation of (30) we used that the contribution of \( \tilde{f} \) to \( E_D(\delta) \) is small for \( U \to 0 \), so that \( E_D(\delta) \) is effectively given by its Hartree approximate. Equation (30) shows that \( E(\delta) - E(0) \), including the fluctuations, has the same form as in the Hartree approximation, albeit with renormalized values of the gap parameter \( H_0 \) and the critical density \( \delta_1 \). In particular, it follows from (30) and (7) that the second derivative of \( E(\delta) \) with respect to \( \delta \) is negative for all \( \delta < \delta_1 \), also when fluctuations are taken into account. As a consequence the pure AFM or CDW phases are again unstable. This demonstrates that, if other (e.g., incommensurate) phases do not interfere, phase separation will actually occur in the extended Hubbard model and, hence, that phase separation is not an artifact of the Hartree approximation. The critical concentration of holes below which phase separation occurs is \( \delta_1 = \sqrt{2} \delta_1 \).

B. Incommensurate phases

In order to investigate whether incommensurate phases might interfere with phase separation, one ought to calculate the renormalization factor \( q(v) \) in the incommensurate broken-symmetry phase. In general this is a difficult task. However, in the SDW phase \( (v < \frac{1}{2}) \) and strictly in \( d = \infty \) the problem simplifies somewhat since the Green functions can be expressed as twofold energy integrals (see Appendix B). From this representation one can indeed show that the renormalization factor for the incommensurate phase is identical to the \( q(v) \) value calculated above for the purely AFM phase. As a consequence, the critical concentration \( \delta_2 \) below which incommensurate phases are stable is renormalized by the same factor as \( \delta_1 \) and \( \delta_1 \). The conclusion is therefore that at weak coupling incommensurate phases do not interfere with phase separation, so that the ground state of the extended Hubbard model is in fact phase separated.

V. SUMMARY AND DISCUSSION

To summarize the results: In this paper we studied the phase diagram of the extended Hubbard model away from half filling at weak coupling on a hypercubic lattice in high dimensions \( (d \gg 1) \). In particular, we were interested in the nature of the broken-symmetry state, the critical density of holes \( \delta_c \), and the order parameter \( \Delta(\delta) \). To study symmetry breaking away from half filling we used second order perturbation theory with respect to \( U \) and \( V \). To simulate finite dimensionality \( (d \geq 3) \) we calculated diagrams up to first order in \( 1/d \). Our most important result is that the dominant broken-symmetry state away from half filling is phase separated: It consists of coexisting antiferromagnetic or CDW domains (at density \( n = 1 \)) and homogeneous domains (at density \( n = 1 - \delta_c < 1 \)).

We further found that the phase diagram predicted by the Hartree approximation is qualitatively but not quantitatively correct. Even in the extreme weak-coupling limit \( (U,V \to 0) \), the Hartree results for \( \delta_c \) and \( \Delta(\delta) \) are renormalized by a factor \( q(v) < 1 \). The renormalization factor \( q(v) \) is identical to the renormalization factor found previously\(^{17,18}\) for the same model at half filling. We recall\(^{17,18}\) that the value of \( q(v) \) for the standard Hubbard model \( (V = 0) \) in \( d = 3 \) is approximately given by \( q = 0.282 \), so that the Hartree results are renormalized by a factor of more than 3.

Next I discuss the results. I will address the relevance of our findings for finite dimensions, their relevance for finite values of \( U \) and \( V \), and possible extensions.

Concerning finite dimensionality: Our results for the phase diagram and the critical density of holes have been derived within the framework of a \( 1/d \) expansion. Hence they demonstrate that phase separation occurs in sufficiently high dimensions. Since the occurrence of phase separation is based on a rather subtle comparison of energies for various phases, it is a priori not guaranteed that phase separation still dominates in \( d = 3 \). On the other hand, the \( 1/d \) corrections contained in \( q(v) \) are rather small (especially for \( V = 0 \)), suggesting that the high-dimensional scenario may well survive also in \( d = 3 \). A related issue, requiring further research, is that of the \( 1/d \) corrections in the critical density of holes of the (subdominant) incommensurate phase. A comparison of the \( 1/d \) corrections to \( \delta_2 \) and \( \delta_1 \) could shed additional light on the stability of phase separation in lower dimensions.

Concerning the relevance of our results for finite \( U \) and \( V \): From a simple continuity argument it is immediately clear that the phase separation found here in the weak-coupling limit will be dominant in a finite range of interactions. The size of the phase separation region is a priori unknown. It can, however, be estimated within the Hartree approximation, very similarly to the work on spinless fermions in Ref. 22. One then finds that the incommensurate phases are increasingly favored if the interaction parameters \( U \) and \( V \) increase. From approximately \( 2U \approx 0.5 \) onwards (the precise value depends on \( v \)) incommensurate phases are more stable. This (Hartree) argument shows that the phase separation region in the pure Hubbard model \( (V = 0) \) may well be relatively small, with a critical \( U_c \) of order unity. It would be interesting if \( U_c \) could be observed in the Monte Carlo simulations of the \( d = \infty \) Hubbard model that are presently being carried out. Alternatively, since \( U_c \) appears to be rather small, a reliable estimate could also be obtained in self-consistent second order perturbation theory.

For convenience we assumed (see the Introduction) that the interaction parameters \( U \) and \( V \) are positive, corresponding to Coulomb repulsion. However, it is not difficult to see that our results are in fact valid whenever the ground state of the model at half filling is either antiferromagnetic or a charge density wave. Since we know from Ref. 13 that at half filling the CDW phase is stable in the region \( U < 0 \), \( V > 0 \), while the SDW phase is stable in the region \( U > 0 \), \( V < 0 \) (provided \( |v| \) is not too large), we conclude that our results apply also to these parameter ranges.

As mentioned above, part of future work should be the calculation of \( 1/d \) corrections in the incommensurate phase, the estimate of the critical interaction \( U_c \) above which phase separation is absent, and the comparison of analytical and Monte Carlo results. In particular, for the comparison to
Monte Carlo data it will be necessary to extend the present calculations to positive temperatures. At weak coupling temperature probably does not play an important role: I expect that phase separation dominates, in large parts of the phase diagram and that the Hartree result is renormalized by the same factor $g(v)$ as was found in this paper. However, temperature may become an important parameter for intermediate couplings \([U,V=O(1)]\). Other extensions of the present work could be the study of different phases (e.g., the superconducting phases of the extended Hubbard model for \(U,V<0\)), the study of additional interaction terms in the Hamiltonian, and the study of the influence of phonons or disorder on the stability of phase separation. The hope is that the results of these studies may shed light on possible (tendencies toward) phase separation in real materials and the physical consequences thereof.

ACKNOWLEDGMENTS

It is a pleasure to acknowledge helpful discussions with D. Vollhardt (RWTH Aachen), V. Janiš (Academy of Sciences, Prague), and in particular also with G. Uhrig (Université de Paris-Sud), M. Jarrell (University of Cincinnati), and J. K. Freericks (Georgetown University). This work was supported in part by the Deutsche Forschungsgemeinschaft under SFB 341.

APPENDIX A: THE HARTREE APPROXIMATION (AFM OR CDW PHASE)

For the antiferromagnetic or CDW phases, the Hartree approximation takes the form

\[
n_{i\sigma}^A n_{j\sigma'} \rightarrow \langle n_{i\sigma} \rangle \langle n_{j\sigma'} \rangle - \langle n_{i\sigma} \rangle \langle n_{j\sigma'} \rangle\), \tag{A1}
\]

where the occupation numbers \(\langle n_{i\sigma} \rangle\) are given by (2). The decoupling (A1) leads to a Hartree Hamiltonian of the form

\[
H^H = H_i - \sum_{\sigma,\lambda} \left( h_{\sigma,\lambda} + \mu_0 \right) n_{i\sigma} + \frac{1}{2} \alpha U N \Delta^2 - N(V + \frac{1}{2} U) n^2. \tag{A2}
\]

The operator \(N^H_\lambda\) in (A2) represents the total number of \(\sigma\) spins on the \(\lambda\) sublattice \((\lambda = \pm)\) and \(h_{\sigma,\lambda} = r_{\sigma,0} h_0\) with \(h_0 = \alpha U \Delta\). Furthermore \(\alpha = \frac{1}{2}, r_{\sigma} = \sigma\) in the SDW phase and \(\alpha = 2v - \frac{1}{2}, r_{\sigma} = 1\) in the CDW phase. Equation (A2) differs from the corresponding Hamiltonian at half filling through the factor \(n^2\) in the last term and the appearance of the “effective” chemical potential \(\mu_0\), which is related to \(\mu\) in (1) by

\[
\mu = (2V + \frac{1}{2} U) n + \mu_0. \tag{A3}
\]

The Hamiltonian (A2) is diagonalized as usual by applying a Fourier transformation and a transformation of the form

\[
c_{k\sigma} = a_{k\sigma} d_{k\sigma} + b_{k\sigma} d_{-k-\sigma},
\]

with the constants \(a_{k\sigma}\) and \(b_{k\sigma}\) given by

\[
a_{k\sigma} = \text{sgn}(h_{\sigma}) \sqrt{\frac{\eta_{k\sigma} + \varepsilon_k}{2 \eta_{k\sigma}}}, \quad b_{k\sigma} = \text{sgn}(\varepsilon_k) \sqrt{\frac{\eta_{k\sigma} - \varepsilon_k}{2 \eta_{k\sigma}}}.
\]

As for the half-filled case the eigenenergies of the Hartree Hamiltonian have the form

\[
\eta_{k\sigma} = \text{sgn}(\varepsilon_k) \sqrt{\varepsilon_k^2 + h_0^2}, \tag{A4}
\]

where \(\varepsilon_k = -\sqrt{2J} \sum_{\mu=1} \cos(k_\mu)\) is the dispersion of the noninteracting model. The diagonalized form of (A2) is thus given by

\[
H^H = \sum_{k\sigma} \left( \eta_{k\sigma} - \mu_0 \right) n_{k\sigma} + \frac{1}{2} \alpha U N \Delta^2 - N(V + \frac{1}{2} U) n^2, \tag{A5}
\]

where \(n_{k\sigma} = d_{k\sigma}^\dagger d_{k\sigma}\).

To determine consistency relations for the particle density and the order parameter one needs the Green functions for the \(c_{k\sigma}\) particles (in position space). These can be written as linear combinations of the Green functions of the \(d_{k\sigma}\) particles, which are given by

\[
\langle T \delta_{d_{k\sigma}}(\tau) \delta_{d_{k\sigma}}^\dagger(\tau') \rangle = \delta_{\tau,\tau'} g_{k\sigma}(\tau - \tau'), \tag{A6}
\]

\[
g_{k\sigma}(\tau) = e^{-(\eta_{k\sigma} - \mu_0)\tau} \left[ \theta(\tau - 0^+) \left( 1 - \langle n_{k\sigma} \rangle \right) - \theta(0^+ - \tau) \langle n_{k\sigma} \rangle \right].
\]

In the limit \(d \rightarrow \infty\) the Green functions for the \(c_{k\sigma}\) particles can be reduced to one-dimensional energy integrals. With the definition \(/ = |l| = \sum_{n=-1}^\infty |\xi_n|\) for the length of \(l\) on the lattice one finds that \((T c_{l+1,\sigma}(\tau) c_{l\sigma}^\dagger(0))\) takes the form

\[
G_{\lambda,\sigma}(\tau) = P_{\lambda,\sigma}(\tau,\beta) = -\lambda h_{\sigma} Q_{\lambda,\sigma}(\tau,\beta), \tag{A7}
\]

where by definition \(j \in \lambda\) sublattice. The functions \(P_{\lambda,\sigma}(\tau,\beta)\) and \(Q_{\lambda,\sigma}(\tau,\beta)\) for the doped case \((n<1)\) are given by the same expressions as for \(n=1:\)

\[
P_{\lambda,\sigma}(\tau,\beta) = (2d)^{-\gamma/2} \int_0^{\infty} \, d\varepsilon \nu_\beta(\varepsilon) \text{He}_\lambda(\varepsilon) \left[ g_{\lambda}(\tau) + g_{-\lambda}(\tau) \right],
\]

\[
Q_{\lambda,\sigma}(\tau,\beta) = (2d)^{-\gamma/2} \int_0^{\infty} \, d\varepsilon \nu_\beta(\varepsilon) \text{He}_\lambda(\varepsilon) \left[ g_{\lambda}(\tau) - g_{-\lambda}(\tau) \right],
\]

if \(\gamma\) is even and

\[
P_{\lambda,\sigma}(\tau,\beta) = - (2d)^{-\gamma/2} \int_0^{\infty} \, d\varepsilon \nu_\beta(\varepsilon) \times \text{He}_\lambda(\varepsilon) \left[ g_{\lambda}(\tau) - g_{-\lambda}(\tau) \right],
\]

\[
Q_{\lambda,\sigma}(\tau,\beta) = 0,
\]

if \(\gamma\) is odd. Note, however, that the symmetry properties of \(P_{\lambda,\sigma}\) and \(Q_{\lambda,\sigma}\) as a function of \(\tau\) are different from those for the half-filled case due to the different form of \(g_{\lambda}(\tau)\) in (36).

The above expressions for the on-site and nearest neighbor Green functions \((\gamma = 0,1)\) hold in all dimensions \(d\), not just in \(d=\infty\). Concerning the notation: \(\text{He}_\lambda(\varepsilon)\) is a Hermite polynomial and \(\nu_\beta(\varepsilon)\) is the density of states for the noninteracting model \((U = V = 0)\).

In the following we consider only the ground state \((T=0)\), where the average number of \(d_{k\sigma}\) particles is simply
given by \( \langle \nu_{\sigma} \rangle = \delta (\mu_0 - \eta_\sigma) \). Hence the Hartree ground state energy per site \( E(\delta) \) at a given concentration of holes \( \delta = 1 - n \) follows from (A5) as

\[
E(\delta) = \frac{1}{2} \alpha U \Delta^2 + \left( V + \frac{1}{2} U \right) n^2 - 2 \int_{\varepsilon_m}^{\infty} d\varepsilon \nu_d(\varepsilon) \eta_\varepsilon ,
\]

(A8)

where \( \varepsilon_m \) is defined as \( \varepsilon_m = \sqrt{\mu_0^2 - h_0^2} \). In (A8) we assumed \( n < 1 \), or \( \delta > 0 \). The concentration of holes is obviously given by

\[
\delta = 2 \int_{\varepsilon_m}^{\infty} d\varepsilon \nu_d(\varepsilon) .
\]

(A9)

This equation could alternatively be derived from the consistency relation \( n_\sigma = -\frac{1}{2} \Sigma_x G_{0\sigma}(0) \). Similarly, the order parameter \( \Delta \) follows from the consistency relation \( \Delta = -\Sigma_x \lambda G_{0\uparrow}(0) \). One finds that either \( \Delta = 0 \) (which is the solution in the homogeneous phase) or

\[
1 = 2 \alpha U \int_{\varepsilon_m}^{\infty} d\varepsilon \nu_d(\varepsilon) / \eta_\varepsilon .
\]

(A10)

The critical concentration of holes \( \delta_1 \) is defined by \( \Delta(\delta_1) = 0 \) and satisfies the equation

\[
1 = 2 \alpha U \int_{\varepsilon_m}^{\infty} d\varepsilon \nu_d(\varepsilon) / \varepsilon .
\]

(A11)

Below we consider these equations for \( E(\delta), \Delta(\delta) \), and \( \delta_1 \) in the limit of weak coupling.

At weak coupling one expects the order parameter and the critical concentration of holes to be small. In fact, we know already from the calculations at half filling,\textsuperscript{17,18} see (3), that the gap parameter \( H_0 = \alpha U \Delta(0) \) for \( n = 1 \) is exponentially small for \( U \downarrow 0 \). Similarly we will find below that \( \delta_1 \) is exponentially small. Anticipating this result we can approximate (A9) at weak coupling by

\[
\delta \sim 2 \nu_d(0) \varepsilon_m \quad (U \downarrow 0) .
\]

(A12)

If one approaches half filling \( (\delta \downarrow 0) \) then \( \varepsilon_m \downarrow 0 \), or \( \mu_0 \downarrow H_0 \). Precisely at half filling one knows that the effective chemical potential \( \mu_0 \) vanishes identically, so that \( \mu_0 \) is necessarily discontinuous at \( \delta = 0 \). Physically this is obvious due to the presence of a gap.

The order parameter \( \Delta(\delta) \) at weak coupling can most easily be determined by subtracting from (A10) the equation for the order parameter at half filling [i.e., Eq. (A10) with \( \varepsilon_m \rightarrow 0 \) and \( h_0 \rightarrow H_0 \)]. This yields

\[
\int_{\varepsilon_m}^{\infty} d\varepsilon \nu_d(\varepsilon) \left[ \frac{1}{\sqrt{\varepsilon^2 + h_0^2}} - \frac{1}{\sqrt{\varepsilon^2 + H_0^2}} \right] = \int_{\varepsilon_m}^{\infty} d\varepsilon \nu_d(\varepsilon) \frac{1}{\sqrt{\varepsilon^2 + h_0^2}}.
\]

If we now define \( r = h_0/H_0 = \Delta(0) \) and \( a = \varepsilon_m / H_0 = \delta / 2 \nu_d(0) H_0 \), we can take the limit \( U \downarrow 0 \), or \( H_0 \downarrow 0 \), to find

\[
\int_{0}^{\infty} dy \left[ \frac{1}{\sqrt{y^2 + r^2}} - \frac{1}{\sqrt{y^2 + 1}} \right] = \int_{0}^{a} dy \frac{1}{\sqrt{y^2 + r^2}}.
\]

The integrals are standard. The result is \( r^2 = 1 - 2a \), which is equivalent to Eq. (5) given in the main text.

Next we calculate the energy gain per site \( E_\delta \) due to symmetry breaking. The energy gain has to be calculated at fixed density, i.e., for fixed \( \varepsilon_m \). It follows from (A8) that

\[
E_\delta(\delta) = \frac{1}{2} \alpha U \Delta^2 - 2 \int_{\varepsilon_m}^{\infty} d\varepsilon \nu_d(\varepsilon) (\eta_\varepsilon - \varepsilon).
\]

If one uses the consistency relation (40) to rewrite the first term on the right as an \( \varepsilon \) integral, \( E_\delta(\delta) \) takes a simpler form:

\[
E_\delta(\delta) = -2 h_0^2 \nu_d(0) \int_{a}^{\infty} dx \left( \frac{1}{\sqrt{x^2 + 1}} - x - \frac{1}{2} \frac{1}{\sqrt{x^2 + 1}} \right)
\]

\[
= -\frac{1}{2} H_0^2 \nu_d(0) \left( 1 - \frac{\delta}{\delta_1} \right)^2 .
\]

This proves the result quoted in Eq. (6). In the last step we used the known dependence of \( r = h_0/H_0 \) and \( a = \frac{1}{2} (1 - r^2) \) on the doping concentration \( \delta \).

The difference between the ground state energy \( E(\delta) \) at concentration \( \delta \) and the ground state energy at half filling follows from (A8) as

\[
E(\delta) - E(0) = (V + \frac{1}{2} U)(n^2 - 1) + \frac{1}{2} \alpha U \Delta^2(\Delta(0))
\]

\[
- 2 \int_{\varepsilon_m}^{\infty} d\varepsilon \nu_d(\varepsilon) \sqrt{\varepsilon^2 + h_0^2}
\]

\[
+ 2 \int_{0}^{\infty} d\varepsilon \nu_d(\varepsilon) \sqrt{\varepsilon^2 + H_0^2}.
\]

This can for small \( U \), or \( H_0 \), be rewritten as

\[
E(\delta) - E(0) = (V + \frac{1}{2} U)(\delta^2 - 2 \delta)
\]

\[
+ 2 \nu_d(0) H_0^2 \left( \int_{0}^{a} dy \sqrt{\frac{y^2 + 1}{y^2 + r^2}} + \int_{0}^{a} dy \sqrt{\frac{y^2 + r^2}{y^2 + 1}} \right).
\]

Since \( \delta = O(H_0) \), the term of order \( U \delta^2 \) in the right hand side can be neglected. The integrals can be calculated in an elementary way. The result is given in Eq. (7).

**APPENDIX B: THE HARTREE-FOCK APPROXIMATION**

**(INCOMMENSURATE PHASES)**

In this appendix we study the broken-symmetry spin density wave phase, characterized by the incommensurate wave vector \( \mathbf{q} \neq \mathbf{Q} \). To obtain explicit results, we focus again on the limit of high dimensions \( d = \infty \).

For general spin density waves of the form (11) the Hartree-Fock decoupling is slightly more complicated than (A1), namely,
The Hamiltonian of the form

\[ H_{\text{eff}} = H_0 - \sum_{\mathbf{k}} \left\{ \left( (h_{\sigma} \cos(q \cdot i) + \mu_0) n_{i\sigma} + c_{i\sigma} c_{\mathbf{k} + q \cdot \mathbf{i} - \mathbf{a}} \sin(q \cdot i) \right) + \frac{1}{2} U N \Delta^2 - N(V + \frac{1}{2} U) n^2 \right\} \]

with \( h_{\sigma} = \sigma h_0 \) and \( h_0 = \frac{1}{2} U \Delta \).

The Hamiltonian (B2) can be diagonalized as follows.\(^{31}\) First define vector operators \( c_i = (c_{i\uparrow}, c_{i\downarrow}) \). The interaction part of (A2) can then be diagonalized with the use of a local canonical transformation \( c_i = T_{\mathbf{k}} \gamma_i \) to new particles \( \gamma_i \). The matrix \( T_{\mathbf{k}} \) is defined as \( T_{\mathbf{k}} = \exp(-i \mathbf{q} \cdot \mathbf{r}_i) \), where \( \sigma_r \) is the second Pauli matrix.\(^{28}\) A Fourier transformation \( \gamma_i = \gamma_{\mathbf{k}} \) then renders the Hamiltonian diagonal in \( \mathbf{k} \) space, but not yet in spin space. To diagonalize the spin degrees of freedom one needs a second transformation \( \mathbf{y}_k = T_{\mathbf{k}} \mathbf{d}_k \) to new particles \( \mathbf{d}_{\mathbf{k} \sigma} \). The matrix \( T_{\mathbf{k}} \) is given by \( T_{\mathbf{k}} = \exp(i \phi_{\mathbf{k} \alpha}) \), where \( \phi_{\mathbf{k}} \) is a Pauli matrix, and the angle \( \phi_{\mathbf{k}} \) (satisfying \( 0 < \phi_{\mathbf{k}} < \pi \)) is defined by \( \cos(\phi_{\mathbf{k}}) = h_0 / \eta_k \) with \( \eta_k = \text{sgn}(B_k) \sqrt{B_k^2 + h_0^2} \), \( B_k = \frac{1}{2} (e_+ + e_-) \), and \( e_\sigma = e_\sigma \eta_k \). The resulting Hamiltonian for the \( \mathbf{d}_{\mathbf{k} \sigma} \) particles has the same form as (A5) for \( \alpha = \frac{1}{2} \), but the eigenenergies \( \eta_k \) are now given by

\[ \eta_k = A_k - \sigma \eta_k \]  

with \( A_k = \frac{1}{2} (e_+ + e_-) \). Hence the ground state energy of the incommensurate phase is given by

\[ E = 2 N^{-1} \sum_k \eta_k \theta(\mu_0 - \eta_k) + \frac{1}{2} U N \Delta^2 + (\frac{1}{2} U + V) n^2, \]

(B4)

where \( \eta_k = \eta_k \). The factor of 2 in the first term is due to the spin summation and \( \theta(x) \) is the Heaviside step function.

Along the lines of Appendix A one can calculate the Green functions of the \( \mathbf{d}_{\mathbf{k} \sigma} \) particles which, for the incommensurate SDW, are nondiagonal in spin space. Since we restrict consideration to \( d = \infty \), it suffices for the calculation of diagrams to determine the Green function for \( \tau \neq 0 \) only. If we define

\[ P_0(\tau) = \frac{1}{N} \sum_k g_{\mathbf{k} \uparrow}(\tau), \quad Q_0(\tau) = -\frac{1}{N} \sum_k g_{\mathbf{k} \downarrow}(\tau) / \eta_k, \]

then the Green function \( G_{\sigma\sigma'}(\tau) = \langle T_{i} c_{i\sigma'}(\tau) c_{i\sigma}(0) \rangle \) can be written as

\[ G_{\sigma\sigma'}(\tau) = \delta_{\sigma\sigma'} [P_0(\tau) - \sigma h_0 \cos(q \cdot i)] Q_0(\tau) \]

where \( h_0 = \sin(q \cdot i) \delta_{\sigma\sigma'} Q_0(\tau) \).

For \( q = Q \) this reduces to (A7) for \( \beta = 0 \).

The consistency relations for the chemical potential and the order parameter (for a given hole density \( \delta \)) follow from \( G_{\sigma\sigma'}(\tau) \) as

\[ \delta = \frac{1}{N} \sum_{\mathbf{k} \sigma} \theta(\eta_{\mathbf{k} \sigma} - \mu_0) \theta(-\eta_{\mathbf{k} \sigma}) \]

and

\[ 1 = \frac{U}{2 N} \sum_{\mathbf{k} \sigma} \theta(\mu_0 - \eta_{\mathbf{k} \sigma}) / \eta_k, \]

respectively. Apart from these two consistency conditions there is a third equation, namely, that for the optimal incommensurability,

\[ \frac{\partial E_0}{\partial \eta_k} = 0. \]

(B7)

Clearly, in view of (B4), Eq. (B7) also has the form of a sum over the first Brillouin zone.

The essential simplification in \( d = \infty \) is that the \( \mathbf{k} \) sums in the above expressions for \( G_{\sigma\sigma'}(\tau) \), \( \delta \), and the optimal incommensurability \( \rho_{\text{opt}} \) can be replaced by twofold integrals involving only the single parameter \( \rho_0 \) defined in (9). In fact in \( d = \infty \) it holds for any function \( F(e_+, e_-) \), with \( e_\sigma \) defined above, that in the thermodynamic limit\(^{35,29}\)

\[ \frac{1}{N} \sum_{\mathbf{k}} F(e_+, e_-) = \int d e_+ \int d e_- g(e_+, e_-; \rho_0) F(e_+, e_-), \]

(B8)

where \( g(e_1, e_2; \rho_0) \) is the bivariate normal probability distribution with correlation coefficient \( \rho_0 \) (see Ref. 30, Chap. 26).

This reduction to twofold integrals in \( d = \infty \) makes the analysis of Eqs. (B5)–(B7) for the density, the order parameter, and the incommensurability tractable. In fact one can show (see Appendix C) that a further simplification occurs in the weak-coupling limit.

**APPENDIX C: SELF-CONSISTENCY EQUATIONS IN THE INCOMMENSURATE PHASE**

In this section we show that the expressions in terms of two-dimensional integrals, derived in Appendix B for the chemical potential, the order parameter, and the optimal incommensurability, can be reduced to relatively simple one-dimensional integrals in the weak-coupling limit. We discuss the relation for the chemical potential in some detail and summarize results for other quantities.

In the case of relation (B5), which fixes the chemical potential as a function of the hole density, we apply (B8) with \( F(e_1, e_2) = \sum_\sigma \theta(\mu_0 - \eta_\sigma(e_1, e_2)) \) and find

\[ \delta = 2 \int de_1 \int de_2 g(e_1, e_2; \rho_0) \theta[-\eta(e_1, e_2)] \]

\[ \times \theta(\eta(e_1, e_2) - \mu_0). \]

(C1)

Here the right hand side is obtained by using the symmetry property \( \eta(-e_1, -e_2) = -\eta(e_1, e_2) \). Equation (C1) shows that \( n = 1 \Leftrightarrow \mu_0 = 0 \) and \( n < 1 \Leftrightarrow \mu_0 < 0 \).
The reduction of (C1) to a one-dimensional integral is greatly simplified if one transforms from the energy variables \((e_1, e_2)\) to new variables \((A, B)\), where \(A = \frac{1}{2} (e_1 + e_2)\) and \(B = \frac{1}{2} (e_1 - e_2)\) have been defined near \((B3)\). The advantage of the \((A, B)\) variables is that the two-particle density of states is diagonal in \(A\) and \(B\), so that

\[
\delta = \frac{1}{\pi \sqrt{\kappa (1 - \kappa)}} \int 2 \left| A \right| dA \int 2 \left| B \right| dB \exp \left[ - \frac{A^2}{2 \kappa} - \frac{B^2}{2 (1 - \kappa)} \right] 
\]

\[
\times \partial (-A + \eta) \partial (-A - \eta - \mu_0) 
\]

\[
= \frac{1}{\pi \sqrt{\kappa (1 - \kappa)}} \int_0^\infty 2 \left| A \right| dA \exp \left[ - \frac{B^2}{2 (1 - \kappa)} \right] 
\]

\[
\times \int_0^\infty \left| \frac{- \mu_0 + \eta}{\mu_0 + \eta} \right| dA \exp \left[ - \frac{A^2}{2 \kappa} \right].
\]

(C2)

Here \(\kappa = (1 + \rho_0)/2\) contains the entire \(q\) dependence. It is now advantageous to introduce rescaled variables \(\alpha = \sqrt{2 \kappa} A\), \(\beta = B/\sqrt{2 \kappa}\), \(s = -\mu_0/\sqrt{2 \kappa}\), and \(g = h_0/\sqrt{2 \kappa}\), since for the optimal incommensurate phase \(\alpha\), \(\beta\), \(s\), and \(g\) remain finite in the limit \(U \to 0\). Note that the rescaled chemical potential \(\rho\) and the rescaled order parameter \(g\) are both positive. In terms of these new variables,

\[
\delta = \frac{2}{\pi \sqrt{\kappa}} \int_0^\infty d\beta e^{-\kappa \beta^2/(1 - \kappa)} \int_{-\infty}^\infty d\alpha e^{-\alpha^2},
\]

(C3)

where \(\alpha \pm \beta = \sqrt{\beta^2 + g^2} \pm s\). For large \(\beta\) (i.e., \(\beta \gg s\)), the \(\alpha\) integral in (C1) takes the form \(e^{-\alpha^2}/2\alpha\), so that the \(\beta\) integral converges rapidly on a scale \(\beta = O(1)\). This implies that for \(U \to 0\), where \(\kappa \to 0\), one can replace the factor \(e^{-\kappa \beta^2/(1 - \kappa)}\) by unity. This yields

\[
\delta \sim \frac{2}{\pi \sqrt{\kappa}} \int_0^\infty d\beta \int_{-\infty}^\infty d\alpha e^{-\alpha^2} (U \to 0).
\]

This integral, which is still two-dimensional, can simply be reduced to a one dimensional integral by changing the order of integration. After a few elementary manipulations the end result can then be written as

\[
\delta \sim \frac{4}{\pi \sqrt{\kappa}} \int_0^\infty d\alpha \sqrt{\alpha^2 - g^2} e^{-\alpha^2 - s^2} \sinh(2s\alpha) \quad (U \to 0).
\]

(C4)

The relations (C4)--(C6) form a closed set of equations for \(s\), \(g\), and \(g_0\), or, equivalently, for the chemical potential \(\mu_0\), the order parameter \(\Delta\), and the incommensurability parameter \(\kappa\).

Once the equilibrium values of the chemical potential \(\mu(\delta)\), the order parameter \(\Delta(\delta)\) and the incommensurability \(\kappa(\delta)\) are known as functions of the doping concentration, one can continue and calculate thermodynamic properties, such as the ground state energy. Again, the ground state energy \(E(\delta)\) can be cast into a relatively simple form involving only one-dimensional integrals. One finds that

\[
E(\delta) = E(0) + \nu(0) \left[ \kappa_{\text{opt}} + 2H^2_0F_1(r^2) \right] + \left( \frac{1}{4} U + V \right) (\delta^2 - 2 \delta) + T,
\]

where \(\Delta = \Delta(\delta)/\Delta_0\), \(F_1(x) = \frac{x}{4} \left[ 1 - x + x \ln(x) \right]\), and

\[
T = - \frac{2 \sqrt{2}}{\pi} \kappa \int_0^\infty dy e^{-y^2 - s^2} \cosh(2ys) \left[ \frac{y}{\sqrt{y^2 - g^2}} - y \sqrt{y^2 - g^2} \right]
\]

\[
- g^2 \sinh \left( \frac{y}{g} \sqrt{\frac{y^2}{g^2} - 1} \right).
\]

The relation (C7), in combination with (C4)--(C6), is the starting point for analytical and numerical work in the incommensurate phase at weak coupling.
16 Here we discuss only the SDW phase ($v < \frac{1}{2}$). The CDW phase is technically more difficult, yet one expects that the physics (i.e., the conclusion that phase separation dominates) is the same for the SDW and CDW phases.
20 The calculations are very similar, but by no means identical, to those for the half-filled case. The main differences result from the presence of the effective chemical potential $\mu_0$, which introduces both an energy cutoff ($\mu_0$) and a characteristic time scale ($1/\mu_0$) into the problem.